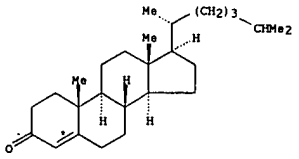
=> d ibib ab fhit 1-3

L6 ANSWER 3 OF 3 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER: 116:152142 CASREACT
TITLE: Oxidation of natural targets by dioxiranes. Oxyfunctionalization of steroids
AUTHOR(S): Bovicelli, Paolo; Lupattelli, Paolo; Mincione, Enrico; Prencipe, Teresa; Curci, Ruggero
CORPORATE SOURCE: Dep. Chem., Univ. Rome "La Sapienza", Rome, I-00185, Italy
SOURCE: Journal of Organic Chemistry (1992), 57(7), 2182-4
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English

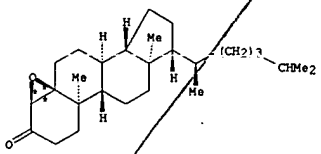
AB The oxyfunctionalization of 4-unsatd. steroids I (R = C8H17, Ac) with dimethyldioxirane (II) gave 80-90% 4,5-epoxides III with .alpha.:.beta. = 3:1 and 4:1, resp. The treatment of 5,16-pregnandien-20-one IV with II gave 95% 5,6-epoxide V with .beta.:.alpha. = 3:2. The treatment of 1,4-unsatd. steroid VI with II gave 80% 1,2-epoxide VII. The oxidn. of estrone acetate with II gave the corresponding 9.alpha.-hydroxy deriv.

RX(1) OF 4 2 A ===> B + C

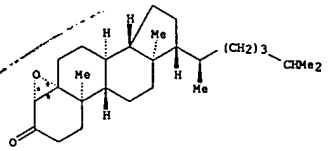


2 A

(1)



B
YIELD 80%(75)



C
YIELD 80%(25)

RX(1) RCT A 601-57-0
RGT D 74087-85-7 Dimethyldioxirane
PRO B 2515-12-0, C 1975-34-4
SOL 67-64-1 Me2CO

L6 ANSWER 3 OF 3 CASREACT COPYRIGHT 2003 ACS (Continued)

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=>
Uploading 627.str

L7      STRUCTURE UPLOADED

=> s l7 full
FULL SEARCH INITIATED 09:07:52 FILE 'CASREACT'
SCREENING COMPLETE -  11165 REACTIONS TO VERIFY FROM   1460 DOCUMENTS

100.0% DONE  11165 VERIFIED     405 HIT RXNS                    154 DOCS
SEARCH TIME: 00.00.01

L8          154 SEA SSS FUL L7 (   405 REACTIONS)

=> d his

     (FILE 'HOME' ENTERED AT 09:00:53 ON 07 MAR 2003)

     FILE 'CASREACT' ENTERED AT 09:01:03 ON 07 MAR 2003
L1              STRUCTURE UPLOADED
L2            7 S L1
L3          154 S L1 FULL
L4          134 S L3 NOT PY>=2000

     FILE 'REGISTRY' ENTERED AT 09:03:39 ON 07 MAR 2003
L5          106 S DIOXIRANE

     FILE 'CASREACT' ENTERED AT 09:04:10 ON 07 MAR 2003
L6            3 S L3 AND L5
L7              STRUCTURE UPLOADED
L8          154 S L7 FULL

=> s l8 and l5
          541 L5
L9          3 L8 AND L5

=> d ibib ab fhit 1-14
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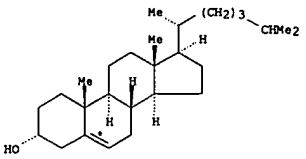
L11 ANSWER 1 OF 14 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 134:29610 CASREACT
TITLE: Highly .beta.-selective epoxidation of .DELTA.5-unsaturated steroids catalyzed by ketones
AUTHOR(S): Yang, Dan; Jiao, Guan-Sheng
CORPORATE SOURCE: Department of Chemistry, The University of Hong Kong, Hong Kong, Peop. Rep. China
SOURCE: Chemistry--A European Journal (2000), 6(19), 3517-3521
CODEN: CEUJED; ISSN: 0947-6539
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A general catalytic and environmentally friendly method for .beta.-epoxidn. of .DELTA.5-unsatd. steroids has been developed, which uses ketones as the catalysts and Oxone as the terminal oxidant. A whole range of .DELTA.5-unsatd. steroids, which bear different functional groups such as hydroxyl, carbonyl, acetyl, or ketal, as well as different side chains, were conveniently converted to the corresponding synthetically and biol. interesting 5.beta.,5.beta.-epoxides with excellent .beta.-selectivities and high yields.

RX(1) OF 21 A ===> B

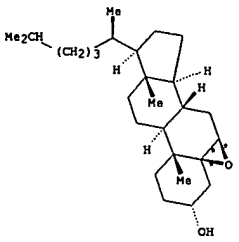


A

(1)

10/2000

L11 ANSWER 1 OF 14 CASREACT COPYRIGHT 2003 ACS (Continued)



B
YIELD 90%

RX(1) RCT A 474-77-1

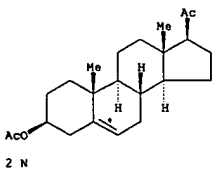
STAGE(1)
RGT C 67-64-1 Me2CO
SOL 110-71-4 (CH2OMe)2, 75-05-8 MeCN

STAGE(2)
RGT D 139-33-3 Di-Na EDTA
SOL 7732-18-5 Water

STAGE(3)
RGT E 37222-66-5 Oxone, F 144-55-8 NaHCO3
PRO B 24116-45-8
NTE stereoselective (3:1 beta:alpha)
REFERENCE COUNT: 79 THERE ARE 79 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

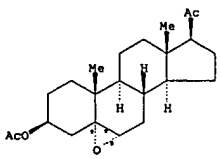
L11 ANSWER 2 OF 14 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 125:143127 CASREACT
TITLE: The study of epoxidation of steroidal alkenes with potassium permanganate-inorganic salts
AUTHOR(S): Parish, Edward J.; Li, Shengrong
CORPORATE SOURCE: Dep. Chem., Auburn Univ., Auburn, AL, 36849, USA
SOURCE: Journal of Chemical Research, Synopses (1996), (6), 288-289
CODEN: JRPSDC; ISSN: 0308-2342
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB CuSO4 could be substituted by other transition metal salts with non-coordinating anions in the .beta.-epoxidn. of steroidal alkenes with KMnO4-CuSO4, which suggested the face selectively might result from the initial formation of a copper-double bond .pi.-complex on the less hindered side. Cholesterol 3-benzoate and 3.beta.-acetoxyprogest-5-en-20-one were reacted with KMnO4 and CuSO4 to form the corresponding 5.beta.,6.beta.-epoxides with high yield and high diastereoselectivity. Similar results were obtained when Cu(NO3)2, NiSO4, Ni(NO3)2, Co(NO3)2, Fe2(SO4)3, Fe(NO3)3, ZnSO4 or Ce(NO3)3 were substituted for CuSO4. When main group metal salts or transition metal salts, such as Co(NO3)2, MgSO4, or Al2(SO4)3, were substituted for copper sulfate, the reaction failed.

RX(9) OF 16 2 N ===> O + P

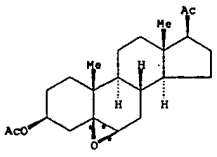


2 N

(9)



O
YIELD 84%(10)



P
YIELD 84%(90)

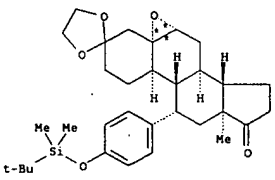
L11 ANSWER 2 OF 14 CASREACT COPYRIGHT 2003 ACS (Continued)

RX(9) RCT N 1778-02-5
RGT D 7722-64-7 KMnO4
PRO O 14148-09-5, P 6661-94-5
CAT 7758-99-8 CuSO4.5H2O
SOL 75-65-0 t-BuOH
NTE stereoselective

L11 ANSWER 5 OF 14 CASREACT COPYRIGHT 2003 ACS (Continued)
SOL 75-09-2 CH2Cl2

STAGE(2)
RGT F 75-65-0 t-BuOH
PRO M 6661-94-5, N 14148-09-5
NTE STEREOSELECTIVE

L11 ANSWER 6 OF 14 CASREACT COPYRIGHT 2003 ACS (Continued)

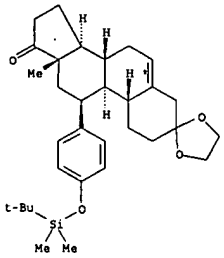


D
YIELD 82%

RX(2) RCT C 156352-58-8
RGT E 7722-84-1 H2O2, F 657-15-8 Ethanone, 2,2,2-trifluoro-1-(3-nitrophenyl)-, G 144-55-8 NaHCO3
PRO D 156352-59-9
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
NTE stereoselective

L11 ANSWER 6 OF 14 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 121:109371 CASREACT
TITLE: Synthesis and biological activity of 17-chloro-16(17)-unsaturated D-homo antiprogestins
AUTHOR(S): Schwede, Wolfgang; Cleve, Arwed; Neef, Guenter; Ottow, Eckhard; Stoeckemann, Klaus; Wiechert, Rudolf
CORPORATE SOURCE: Res. Lab., Schering AG, Berlin, Germany
SOURCE: Steroids (1994), 59(3), 176-80
CODEN: STEDAM; ISSN: 0039-128X .
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An efficient approach to 17-chloro-16(17)-unsatd. D-homo antiprogestins I (Y = Ac, 3-pyridyl) is described. The key steps of the synthesis are a ring-expansion via dichlorocarbene addn. to 17-silyl enol ether II (TBDMS = tert-butyldimethylsilyl) to give D-homosteroid III and a palladium-catalyzed coupling of 11.beta.-(4-aryltriflate) IV with tributyl(1-ethoxyethenyl)stannane or diethyl(3-pyridinyl)borane to give, after deketalization, I (Y = Ac and 3-pyridyl, resp.). The new progesterone antagonists were tested for their biol. activities and compared to those of know antiprogestins.

RX(2) OF 24 ...C ===> D...



C

L11 ANSWER 7 OF 14 CASREACT COPYRIGHT 2003 ACS
ACCESSION NUMBER: 117:212781 CASREACT
TITLE: Catalytic .beta.-stereospecific epoxidation of unsaturated steroids by trans-dioxoruthenium(VI)tetramesitylporphyrin. Stereochemical grounds for the .beta.-diastereofacial selection
AUTHOR(S): Tavares, Manuella; Ramasseul, Rene; Marchon, Jean Claude; Bachet, Bernard; Brassy, Claude; Mornon, Jean Paul
CORPORATE SOURCE: Lab. Chim. Coord., Cent. Etud. Nucl. Grenoble, Grenoble, 38041, Fr.
SOURCE: Journal of the Chemical Society, Perkin Transactions 2: Physical Organic Chemistry (1972-1999) (1992), (8), 1321-9
CODEN: JCPKBH; ISSN: 0300-9580
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The catalytic epoxidn. by dioxygen with trans-dioxoruthenium(VI)tetramesitylporphyrin (I) of the acetic esters of cholesterol, 3-epicholesterol and isocholesterol, as well as of the 7.alpha.-epimer of the latter, is .beta.-stereospecific. Substitution by a Me group on C-6 of pregnenolone acetate results in reduced reactivity towards catalytic epoxidn. and lower .beta.-stereoselectivity. 19-Norsterol esters bearing a double bond at C-8-C-14 or C-14-C-15, e.g., II and III are inert towards epoxidn. catalyzed by I. The variable reactivity of these sterol ester substrates is explained by a transition state in which the steroid nucleus approaches the ruthenium-oxo bond approx. perpendicular to the porphyrin ring. The .beta.-selectivity of .DELTA.5-sterol ester epoxidn. is accounted for in terms of this transition state geometry which provides a good fit between the porphyrin catalyst and the steroid substrate when the .beta.-side faces the oxo ligand. On the other hand, reaction on the .alpha.-side involves unfavorable steric interactions between axial hydrogen atoms on C-3 and C-7 of the substrate and the porphyrin ring and a mesityl substituent of the catalyst, resp. The crystal and mol. structures of cholesteryl Et carbonate and of its 5,6.beta.-epoxide have been detd. by single-crystal x-ray diffraction. The overall conformation of the steroid nucleus is nearly planar in the cholesteryl ester, while it is bent at the junction between rings A and B in the 5,6.beta.-epoxide. This change from pseudo-trans-to cis-stereochem. of the A-B ring junction upon epoxidn. is proposed to amplify the .beta.-diastereofacial selection. Variable temp. 1H NMR spectra indicate that in CD2Cl2 soln. the 5,6.beta.-epoxide (not the 5,6.alpha.-epoxide) of the cholesteryl acetate coordinates the ruthenium atom of I with a nearly perpendicular geometry. These results corroborate the orthogonal substrate approach and the steric origin of the .beta.-stereospecificity in I-catalyzed steroid epoxidns.

RX(5) OF 6 3 H ===> O + P + Q

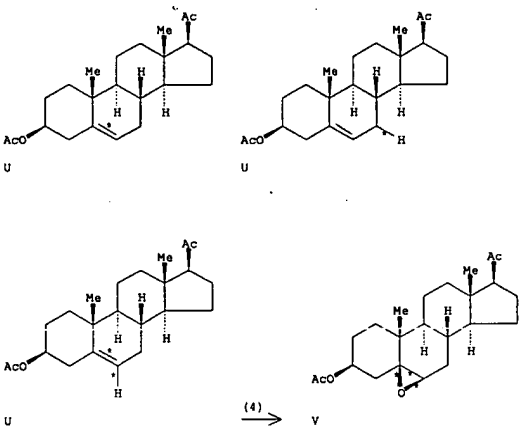
L11 ANSWER 10 OF 14 CASREACT COPYRIGHT 2003 ACS (Continued)

L11 ANSWER 11 OF 14 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER: 112:77709 CASREACT
TITLE: 5.beta.,6.beta.-Epoxidation of 3.beta.-cholesteryl acetate and its analogs
AUTHOR(S): Galagovsky, L. R.; Burton, G.; Gros, E. G.
CORPORATE SOURCE: Fac. Cien. Exactas Nat., Univ. Buenos Aires, Buenos Aires, 1428, Argent.
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1989), 44(7), 806-10
CODEN: ZNBSEN; ISSN: 0932-0776
DOCUMENT TYPE: Journal
LANGUAGE: English

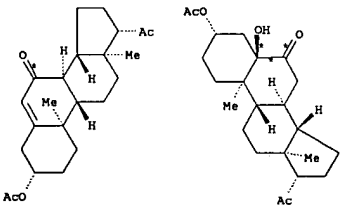
AB The treatment of acetylated .DELTA.5-steroids with chromyl diacetate at low temp. afforded the 5.beta.,6.beta.-epoxy derivs. with stereoselectivity greater than 90 per cent. Thus, the epoxidn. of cholesterol acetate (I) gave 5.beta.,6.beta.-epoxide II as the major product.

RX(4) OF 5 3 U ===> V + W + X



U U U V

L11 ANSWER 11 OF 14 CASREACT COPYRIGHT 2003 ACS (Continued)



W X

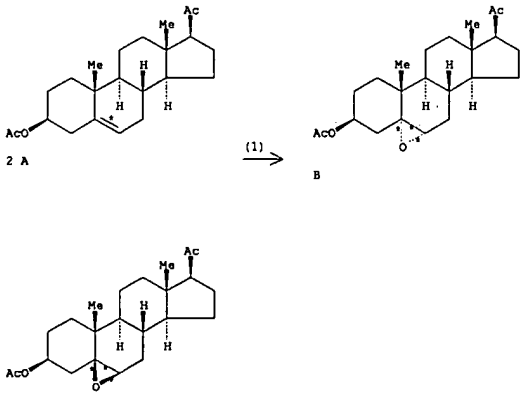
RX(4) RCT U 1778-02-5
RGT E 1333-82-0 CrO3, F 108-24-7 Ac2O
PRO V 6661-94-5, W 6748-09-0, X 2723-04-8
SOL 75-09-2 CH2Cl2

L11 ANSWER 12 OF 14 CASREACT COPYRIGHT 2003 ACS

ACCESSION NUMBER: 109:190646 CASREACT
TITLE: Mercuric oxide - iodine oxidation of 6.beta.-hydroxypregnanes. Influence of the C-5 functionality
AUTHOR(S): Brachet-Cota, Adriana L.; Burton, Gerardo
CORPORATE SOURCE: Fac. Cienc. Exactas Natur., Univ. Buenos Aires, Buenos Aires, 1428, Argent.
SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences (1988), 43(4), 491-5
CODEN: ZNBSEN; ISSN: 0932-0776
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Oxidn. of 6.beta.-hydroxyprogesterone and 3.beta.-acetoxy-5.alpha.,6.beta.-dihydroxypregnan-20-one with mercuric oxide-iodine under photolytic conditions gave 4.alpha.-iodod-5.beta.,6.beta.-oxidopregnan-3,20-dione (I) and 3.beta.-acetoxy-7-iodo-19-formyloxy-5,7-seco-6-norpregnan-5,20-dione (II), resp.

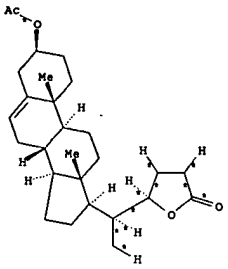
RX(1) OF 17 2 A ===> B + C...



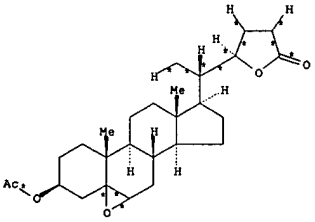
2 A B C

RX(1) RCT A 1778-02-5
RGT D 937-14-4 MCPBA, E 497-19-8 Na2CO3
PRO B 14148-09-5, C 6661-94-5
SOL 7732-18-5 Water, 75-09-2 CH2Cl2

L11 ANSWER 14 OF 14 CASREACT COPYRIGHT 2003 ACS (Continued)



M



N

RX(1) RCT A 2786-02-9, B 145-13-1

STAGE(1)

STAGE(2)
RGT D 104-15-4 TsOH
PRO C 98087-14-0

RX(2) RCT C 98087-14-0

L11 ANSWER 14 OF 14 CASREACT COPYRIGHT 2003 ACS (Continued)

STAGE(1)
RGT G 1333-74-0 H2
CAT 7440-05-3 Pd

STAGE(2)
RCT E 108-24-7
SOL 110-86-1 Pyridine
PRO F 98087-15-1

RX(3) RCT F 98087-15-1
RGT G 1333-74-0 H2
PRO J 98087-16-2, K 98087-17-3
CAT 7440-16-6 Rh

RX(4) RCT J 98087-16-2
RGT O 20427-56-9 RuO4
PRO M 95042-55-0, N 98087-19-5

=> d ibib ab hitstr 1-8

L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2003:58836 CAPLUS
DOCUMENT NUMBER: 138:122759
TITLE: Preparation of 5.beta.,6.beta.-epoxides of steroids by a highly .beta.-selective epoxidation of .DELTA.5-unsaturated steroids catalyzed by ketones
INVENTOR(S): Yang, Dan; Jiao, Guan-Sheng
PATENT ASSIGNEE(S): Hong Kong
SOURCE: U.S. Pat. Appl. Publ., 60 pp., Cont.-in-part of U.S. Ser. No. 788,201, abandoned.
CODEN: USXXCO
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2003018188	A1	20030123	US 2002-91627	20020306
PRIORITY APPLN. INFO.:			US 2000-183396P P	20000218
			US 2001-788201 B2	20010216

OTHER SOURCE(S): MARPAT 138:122759

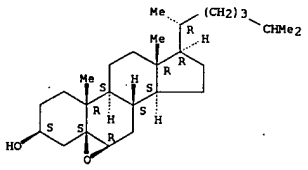
AB The present invention discloses a general, efficient, and environmentally friendly method for epoxidn. of .DELTA.5-unsatd. steroids, such as I [X = H, OH, alkyloxy, acyloxy, silyloxy, CN, carboxy; R1 = H, OH, alkyloxy, aryloxy, halo, CF3, C2F5; R2, R3 = H, alkyl, aryl, halo, OH, alkyloxy, silyloxy; R1R2 = O, ketal; R4, R5 = H, alkyl, halo, OH, alkyloxy, acyloxy, silyloxy; R6, R7 = H, alkyl, halo, OH, alkyloxy, acyloxy], to produce mostly 5.beta.,6.beta.-epoxysteroids II, using certain ketones, such as III [Y = (CR19R20)n, O, S, SO, SO2, amino, alkylamino, arylamino; R11-R14 = H, alkyl, aryl, OH, alkyloxy, aryloxy, acyloxy, silyloxy, halo; R15-R18 = H, alkyl, aryl, carboxy; R19, R20 = H, alkyl, aryl; n = 1-5], as the catalyst along with an oxidizing agent, or by using certain dioxiranes. Thus, to a soln. of cholesterol and ketone (IV) in dimethoxymethane and acetonitrile was added an aq. Na2.EDTA soln. followed by addn. of oxone and sodium bicarbonate, which on usual workup, afforded 5.beta.,6.beta.-epoxycholestan-3.beta.-ol(82% yield).

IT **157-26-6DP**, Dioxirane, derivs.
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(generated in situ from a ketone and an oxidizing agent in prepn. of 5.beta.,6.beta.-epoxides of steroids by .beta.-selective epoxidn. of .DELTA.5-unsatd. steroids catalyzed by ketones)

RN 157-26-6 CAPLUS
CN Dioxirane (9CI, 9CI) (CA INDEX NAME)

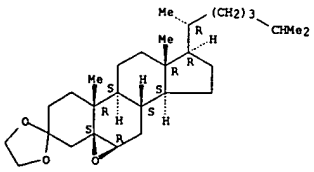
IT **1250-95-9P 2953-38-0P 4025-59-6P 6215-57-2P 6557-20-6P 6585-70-2P 10338-34-8P 14456-17-8P 14733-13-2P 24116-45-8P 29752-14-5P 31081-85-3P 70214-36-7P 71379-18-5P 117884-67-0P**

L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS (Continued)



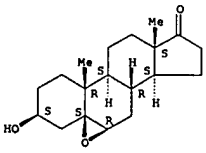
RN 6215-57-2 CAPLUS
CN Cholestan-3-one, 5,6-epoxy-, cyclic 1,2-ethanediyl acetal, (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 6557-20-6 CAPLUS
CN Androstan-17-one, 5,6-epoxy-3-hydroxy-, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



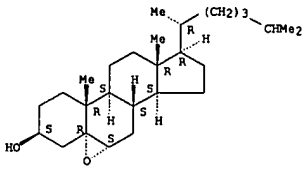
RN 6585-70-2 CAPLUS
CN Pregnan-20-one, 5,6-epoxy-3-hydroxy-, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS (Continued)
119525-36-9P 123153-12-8P 312490-18-9P 312490-19-0P 312490-20-3P 488721-74-0P 488721-75-1P
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)
(prepn. of 5.beta.,6.beta.-epoxides of steroids by .beta.-selective epoxidn. of .DELTA.5-unsatd. steroids catalyzed by ketones)

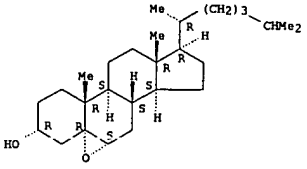
RN 1250-95-9 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, (3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 2953-38-0 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, (3.alpha.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

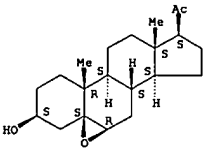
Absolute stereochemistry.



RN 4025-59-6 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

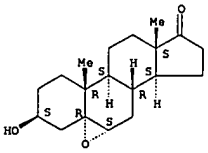
Absolute stereochemistry.

L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS (Continued)



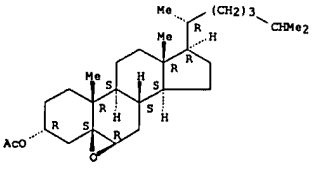
RN 10338-34-8 CAPLUS
CN Androstan-17-one, 5,6-epoxy-3-hydroxy-, (3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 14456-17-8 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, acetate, (3.alpha.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

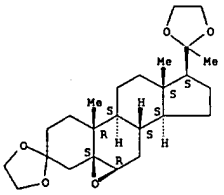
Absolute stereochemistry.



RN 14733-13-2 CAPLUS
CN Pregnane-3,20-dione, 5,6-epoxy-, cyclic bis(1,2-ethanediyl acetal), (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

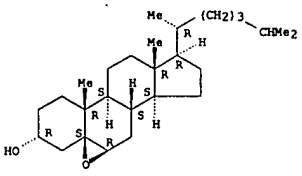
Absolute stereochemistry.

L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS (Continued)



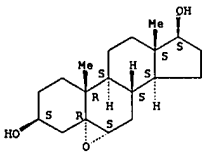
RN 24116-45-8 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, (3.alpha.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 29752-14-5 CAPLUS
CN Androstane-3,17-diol, 5,6-epoxy-, (3.beta.,5.alpha.,6.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

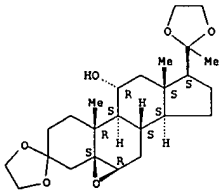


RN 31081-85-3 CAPLUS

L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS (Continued)

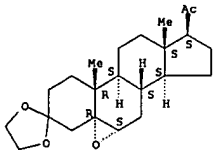
RN 117884-67-0 CAPLUS
CN Pregnane-3,20-dione, 5,6-epoxy-11-hydroxy-, cyclic bis(1,2-ethanediyl acetal), (5.beta.,6.beta.,11.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 119525-36-9 CAPLUS
CN Pregnane-3,20-dione, 5,6-epoxy-, cyclic 3-(1,2-ethanediyl acetal), (5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

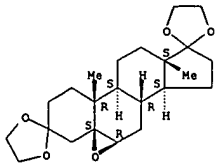


RN 123153-12-8 CAPLUS
CN Pregnane-3,20-dione, 11-(acetyloxy)-5,6-epoxy-, cyclic 3,20-bis(1,2-ethanediyl acetal), (5.beta.,6.beta.,11.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

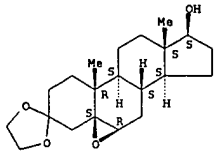
L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS (Continued)
CN Androstane-3,17-dione, 5,6-epoxy-, cyclic bis(1,2-ethanediyl acetal), (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



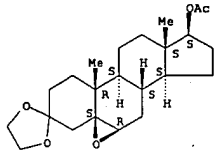
RN 70214-36-7 CAPLUS
CN Androstan-3-one, 5,6-epoxy-17-hydroxy-, cyclic 1,2-ethanediyl acetal, (5.beta.,6.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

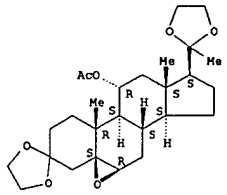


RN 71379-18-5 CAPLUS
CN Androstan-3-one, 17-(acetyloxy)-5,6-epoxy-, cyclic 3-(1,2-ethanediyl acetal), (5.beta.,6.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

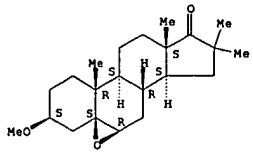


L19 ANSWER 1 OF 8 CAPLUS COPYRIGHT 2003 ACS (Continued)



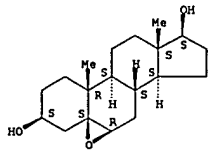
RN 312490-18-9 CAPLUS
CN Androstan-17-one, 5,6-epoxy-3-methoxy-16,16-dimethyl-, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312490-19-0 CAPLUS
CN Androstane-3,17-diol, 5,6-epoxy-, (3.beta.,5.beta.,6.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 312490-20-3 CAPLUS
CN Pregnan-20-one, 5,6-epoxy-3-(methoxymethoxy)-, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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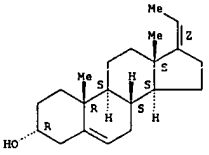
L28 ANSWER 1 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:389246 CAPLUS
DOCUMENT NUMBER: 133:4592
TITLE: Method of epoxidation reaction of olefins
INVENTOR(S): Tian, Weisheng; Yan, Zhaohua
PATENT ASSIGNEE(S): Shanghai Inst. of Organic Chemistry, Chinese Academy of Sciences, Peop. Rep. China
SOURCE: Faming Zhuanli Shenqing Gongkai Shuomingshu, 12 pp.
CODEN: CNXXEV
DOCUMENT TYPE: Patent
LANGUAGE: Chinese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CN 1203915	A	19990106	CN 1998-110882	19980602

PRIORITY APPLN. INFO.: CN 1998-110882 19980602
OTHER SOURCE(S): CASREACT 133:4592
AB Olefins are epoxidized in H2O2-RfSO2F-base oxidn. system and in org. solvent at 0-30.degree.. The mole ratio of olefin-H2O2-RfSO2F-base is 1:2- 12:1-6:2-12, preferably 1:8:4:8. RfSO2F is selected from 2-tetrafluoroethoxytetrafluoroethanesulfonyl fluoride, 2-(2-iodotetrafluoroethoxy)tetrafluoroethanesulfonyl fluoride, 2-(2-chlorotetrafluoroethoxy)tetrafluoroethanesulfonyl fluoride, perfluorooctanesulfonyl fluoride, perfluorobutanesulfonyl fluoride, methoxycarbonyldifluoromethanesulfonyl fluoride, and 2-[2-tetrafluoroethoxy]tetrafluoroethanesulfonyl fluoride; the base from DBU, DBN, NaOEt, NEt3, NaNH2, pyridine, NaOH, KOH, LiOH, Na2CO3, K2CO3, NaOAc, NaHCO3, and KHCO3, etc; and the solvent from THF, EtOH, MeCN, MeOH, and acetone, preferably MeOH.
IT **270251-85-9**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(epoxidn. reaction of olefins)
RN 270251-85-9 CAPLUS
CN Pregna-5,17(20)-dien-3-ol, (3.alpha.,17Z)- (9CI) (CA INDEX NAME)

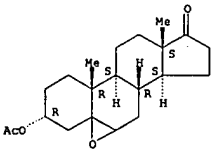
Absolute stereochemistry.
Double bond geometry as shown.



IT **270251-88-2P 270251-89-3P 270251-90-6P**
270251-95-1P 270568-08-6P 270568-09-7P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(epoxidn. reaction of olefins)

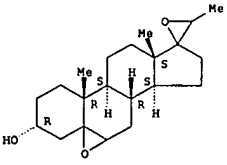
L28 ANSWER 1 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
NAME)

Absolute stereochemistry.



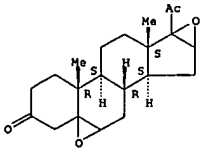
RN 270568-08-6 CAPLUS
CN Pregnan-3-ol, 5,6:17,20-diepoxy-, (3.alpha.,17.xi.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



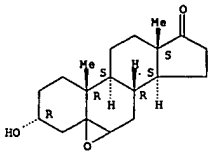
RN 270568-09-7 CAPLUS
CN Pregnane-3,20-dione, 5,6:16,17-diepoxy-, (17.xi.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



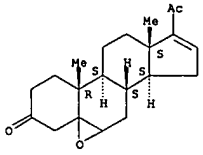
L28 ANSWER 1 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
RN 270251-88-2 CAPLUS
CN Androstan-17-one, 5,6-epoxy-3-hydroxy-, (3.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



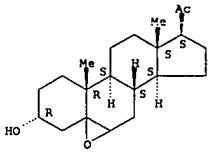
RN 270251-89-3 CAPLUS
CN Pregn-16-ene-3,20-dione, 5,6-epoxy- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 270251-90-6 CAPLUS
CN Pregnan-20-one, 5,6-epoxy-3-hydroxy-, (3.alpha.)- (9CI) (CA INDEX NAME)

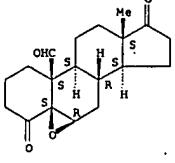
Absolute stereochemistry.



RN 270251-95-1 CAPLUS
CN Androstan-17-one, 3-(acetyloxy)-5,6-epoxy-, (3.alpha.)- (9CI) (CA INDEX

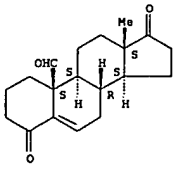
L28 ANSWER 2 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:765906 CAPLUS
DOCUMENT NUMBER: 132:59305
TITLE: Studies of the time-dependent inactivation of aromatase by 4.beta.,5.beta.-epoxy-6-one and 5.beta.,6.beta.-epoxy-4-one steroids under various conditions
AUTHOR(S): Numazawa, Mitsuteru; Yamada, Keiko
CORPORATE SOURCE: Tohoku Pharmaceutical University, Sendai, 981-8558, Japan
SOURCE: Biological & Pharmaceutical Bulletin (1999), 22(11), 1207-1211
CODEN: BPBLEO; ISSN: 0918-6158
PUBLISHER: Pharmaceutical Society of Japan
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The time-dependent inactivation of aromatase by epoxy analogs of the good aromatase inhibitors, androst-4-ene-6,17-dione (3) and androst-5-ene-4,17-dione (7), 4.beta.,5.beta.-epoxy and 5.beta.,6.beta.-epoxy compds. 10 and 13 and their 19-oxo derivs. 11 and 14, was examd. in either the presence or absence of NADPH. The 4.beta.,5.beta.-epoxy-19-oxo steroid 11 along with the 19-methyl-5.beta.,6.beta.-epoxide 13 inactivated human placental aromatase in a mechanism-based manner, in the presence of NADPH, with rate consts. for inactivation (kinact) of 0.133 min-1 for steroid 11 and 0.100 min-1 for steroid 13, whereas the two other steroids, 10 and 14, did not. On the other hand, none of four epoxides studied caused time-dependent inactivation of aromatase in an affinity-labeling manner in the absence of NADPH. These results are the first report showing that inhibitors 11 and 13 are suicide substrates having an epoxyketone structural feature.
IT **253159-01-2P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**
(androstane epoxyketones time-dependent inactivation of aromatase)
RN 253159-01-2 CAPLUS
CN Androstan-19-al, 5,6-epoxy-4,17-dioxo-, (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **244181-97-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(epoxidn. of)
RN 244181-97-3 CAPLUS
CN Androst-5-en-19-al, 4,17-dioxo- (9CI) (CA INDEX NAME)

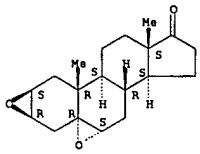
L28 ANSWER 2 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
Absolute stereochemistry.



REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1999:563220 CAPLUS
DOCUMENT NUMBER: 131:337230
TITLE: The transannular effect of one androstane epoxide on the stereochemistry of a second epoxidation
AUTHOR(S): Hanson, James R.; Hitchcock, Peter B.; Kiran, Ismail
CORPORATE SOURCE: Sch. of Chem., Physics and Environmental Science, The University of Sussex, Brighton, BN1 9QJ, UK
SOURCE: Journal of Chemical Research, Synopses (1999), (9), 538-539, 2365-2383
CODEN: JRPSDC; ISSN: 0308-2342
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The transannular directing effect of a 2.alpha.,3.alpha.-, 2.beta.,3.beta.- and 5.alpha.,6.alpha.-epoxide on the epoxidn. of a 5-ene and a 2-ene, resp., is shown to increase the proportion of epoxidn. of the anti face of the alkene when compared to the unsubstituted 2- and 5-androstenes.
IT **249749-39-1P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(crystal structure; transannular effect of one androstane epoxide on the stereochem. of a second epoxidn.)
RN 249749-39-1 CAPLUS
CN Androstan-17-one, 2,3:5,6-diepoxy-, (2.beta.,3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

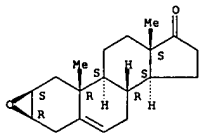
Absolute stereochemistry.



IT **249749-38-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(transannular effect of one androstane epoxide on the stereochem. of a second epoxidn.)
RN 249749-38-0 CAPLUS
CN Androst-5-en-17-one, 2,3-epoxy-, (2.beta.,3.beta.)- (9CI) (CA INDEX NAME)

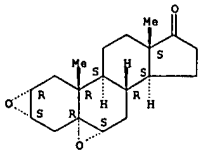
Absolute stereochemistry.

L28 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



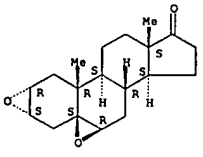
IT **249749-33-5P 249749-36-8P 249749-41-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(transannular effect of one androstane epoxide on the stereochem. of a second epoxidn.)
RN 249749-33-5 CAPLUS
CN Androstan-17-one, 2,3:5,6-diepoxy-, (2.alpha.,3.alpha.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 249749-36-8 CAPLUS
CN Androstan-17-one, 2,3:5,6-diepoxy-, (2.alpha.,3.alpha.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

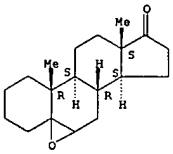
Absolute stereochemistry.



RN 249749-41-5 CAPLUS
CN Androstan-17-one, 5,6-epoxy- (9CI) (CA INDEX NAME)

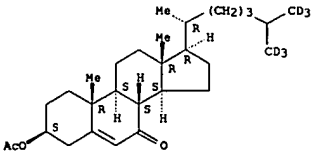
Absolute stereochemistry.

L28 ANSWER 3 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



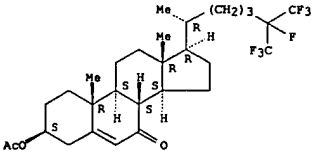
REFERENCE COUNT: 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



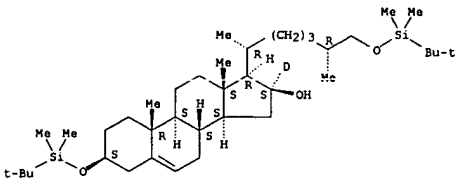
RN 215094-36-3 CAPLUS
CN Cholest-5-en-7-one, 3-(acetyloxy)-25,26,26,26,27,27,27-heptafluoro-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 240129-11-7 CAPLUS
CN Cholest-5-en-16-d-16-ol, 3,26-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, (3.beta.,16.beta.,25R)- (9CI) (CA INDEX NAME)

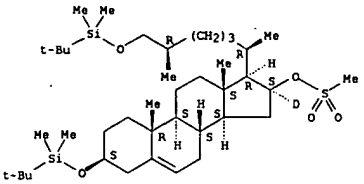
Absolute stereochemistry.



RN 240129-13-9 CAPLUS
CN Cholest-5-en-16-d-16-ol, 3,26-bis[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, methanesulfonate, (3.beta.,16.alpha.,25R)- (9CI) (CA INDEX NAME)

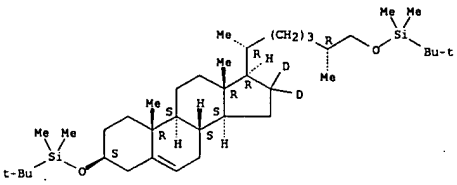
L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.



RN 240129-14-0 CAPLUS
CN Silane, [(3.beta.,25R)-cholest-5-ene-3,26-diyl-16,16-d2-bis(oxy)]bis[(1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

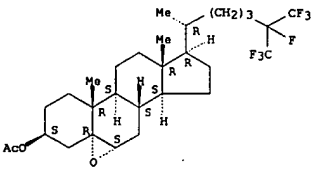
Absolute stereochemistry.



RN 240129-19-5 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-25,26,26,26,27,27,27-heptafluoro-, acetate, (3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

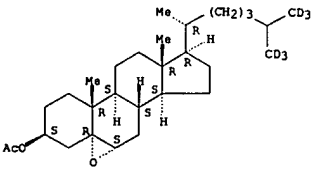
Absolute stereochemistry.

L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



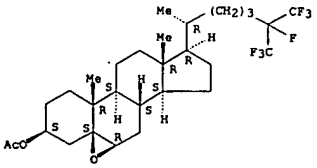
RN 240129-20-8 CAPLUS
CN Cholestan-26,26,26,27,27,27-d6-3-ol, 5,6-epoxy-, acetate, (3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 240129-22-0 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-25,26,26,26,27,27,27-heptafluoro-, acetate, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

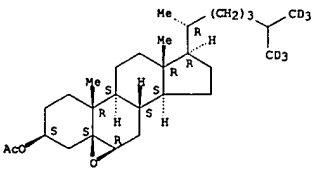
Absolute stereochemistry.



RN 240129-23-1 CAPLUS
CN Cholestan-26,26,26,27,27,27-d6-3-ol, 5,6-epoxy-, acetate, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

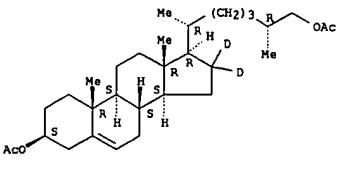
Absolute stereochemistry.

L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



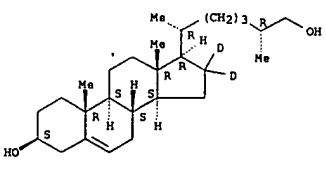
RN 240129-27-5 CAPLUS
CN Cholest-5-ene-16,16-d2-3,26-diol, diacetate, (3.beta.,25R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 240129-28-6 CAPLUS
CN Cholest-5-ene-16,16-d2-3,26-diol, (3.beta.,25R)- (9CI) (CA INDEX NAME)

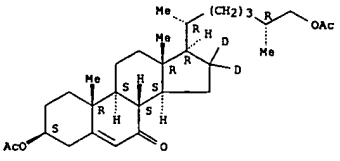
Absolute stereochemistry.



RN 240129-29-7 CAPLUS
CN Cholest-5-en-7-one-16,16-d2, 3,26-bis(acetyloxy)-, (3.beta.,25R)- (9CI) (CA INDEX NAME)

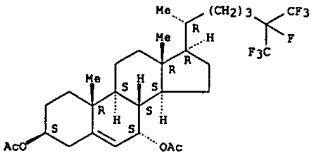
Absolute stereochemistry.

L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



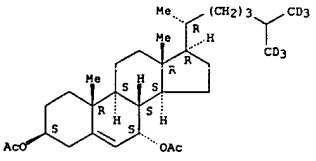
RN 240129-32-2 CAPLUS
CN Cholest-5-ene-3,7-diol, 25,26,26,26,27,27,27-heptafluoro-, diacetate, (3.beta.,7.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 240129-33-3 CAPLUS
CN Cholest-5-ene-26,26,26,27,27,27-d6-3,7-diol, diacetate, (3.beta.,7.alpha.)- (9CI) (CA INDEX NAME)

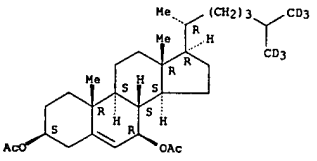
Absolute stereochemistry.



RN 240129-34-4 CAPLUS
CN Cholest-5-ene-3,7,26-triol, triacetate, (3.beta.,7.alpha.,25R)- (9CI) (CA INDEX NAME)

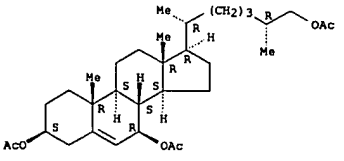
L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.



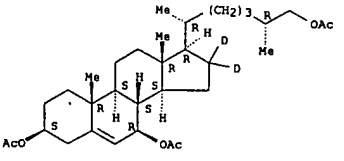
RN 240129-38-8 CAPLUS
CN Cholest-5-ene-3,7,26-triol, triacetate, (3.beta.,7.beta.,25R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 240129-39-9 CAPLUS
CN Cholest-5-ene-16,16-d2-3,7,26-triol, triacetate, (3.beta.,7.beta.,25R)- (9CI) (CA INDEX NAME)

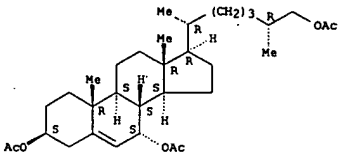
Absolute stereochemistry.



RN 240129-54-8 CAPLUS
CN Cholest-5-ene-3,19-diol, 25,26,26,26,27,27,27-heptafluoro-, 3-acetate, (3.beta.)- (9CI) (CA INDEX NAME)

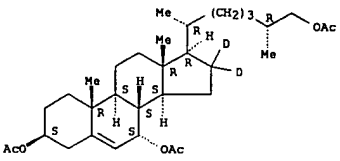
Absolute stereochemistry.

L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
Absolute stereochemistry.



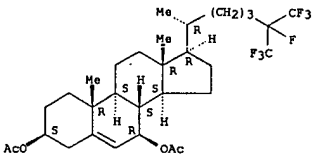
RN 240129-35-5 CAPLUS
CN Cholest-5-ene-16,16-d2-3,7,26-triol, triacetate, (3.beta.,7.alpha.,25R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



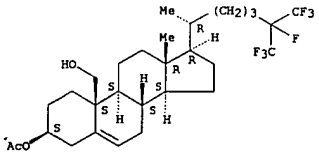
RN 240129-36-6 CAPLUS
CN Cholest-5-ene-3,7-diol, 25,26,26,26,27,27,27-heptafluoro-, diacetate, (3.beta.,7.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



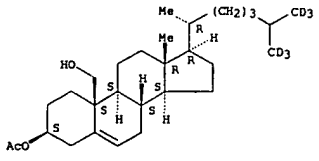
RN 240129-37-7 CAPLUS
CN Cholest-5-ene-26,26,26,27,27,27-d6-3,7-diol, diacetate, (3.beta.,7.beta.)- (9CI) (CA INDEX NAME)

L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



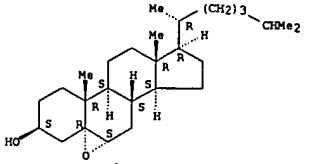
RN 240129-55-9 CAPLUS
CN Cholest-5-ene-26,26,26,27,27,27-d6-3,19-diol, 3-acetate, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



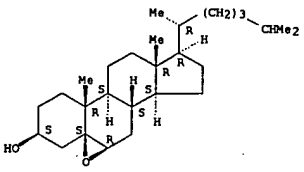
IT **1250-95-9P 4025-59-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and characterization of fluorinated and deuterated analogs of oxygenated derivs. of cholesterol)
RN 1250-95-9 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, (3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 4025-59-6 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

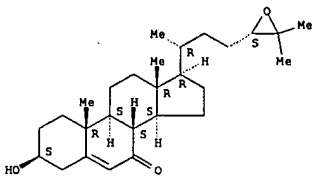
L28 ANSWER 4 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
Absolute stereochemistry.



REFERENCE COUNT: 66 THERE ARE 66 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:809482 CAPLUS
DOCUMENT NUMBER: 130:139506
TITLE: Stereocontrolled syntheses of 24(S),25-epoxycholesterol and related oxysterols for studies on the activation of LXR receptors
AUTHOR(S): Corey, E. J.; Grogan, Michael J.
CORPORATE SOURCE: Department of Chemistry and Chemical Biology, Harvard University, Cambridge, MA, 02138, USA
SOURCE: Tetrahedron Letters (1998), 39(51), 9351-9354
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:139506
AB Efficient syntheses are described of desmosterol, the corresponding 24(S),25 epoxide and various analogs for evaluation as ligands and functional activators of LXR receptors.
IT **220066-66-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **RCT (Reactant)**; SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled syntheses of 24(S),25-epoxycholesterol and related oxysterols for studies on activation of LXR receptors)
RN 220066-66-0 CAPLUS
CN Cholest-5-en-7-one, 24,25-epoxy-3-hydroxy-, (3.beta.,24S)- (9CI) (CA INDEX NAME)

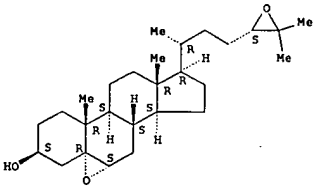
Absolute stereochemistry.



IT **220066-69-3P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**
(stereocontrolled syntheses of 24(S),25-epoxycholesterol and related oxysterols for studies on activation of LXR receptors)
RN 220066-69-3 CAPLUS
CN Cholestan-3-ol, 5,6:24,25-diepoxy-, (3.beta.,5.alpha.,6.alpha.,24S)- (9CI) (CA INDEX NAME)

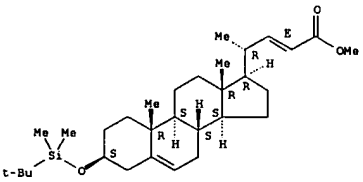
Absolute stereochemistry.

L28 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT **164298-05-9P 220066-72-8P 220150-72-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(stereocontrolled syntheses of 24(S),25-epoxycholesterol and related oxysterols for studies on activation of LXR receptors)
RN 164298-05-9 CAPLUS
CN Chola-5,22-dien-24-oic acid, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, methyl ester, (3.beta.,22E)- (9CI) (CA INDEX NAME)

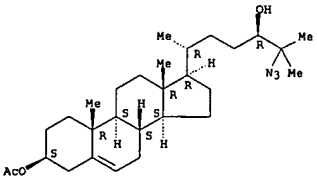
Absolute stereochemistry.
Double bond geometry as shown.



RN 220066-72-8 CAPLUS
CN Cholest-5-ene-3,24-diol, 25-azido-, 3-acetate, (3.beta.,24R)- (9CI) (CA INDEX NAME)

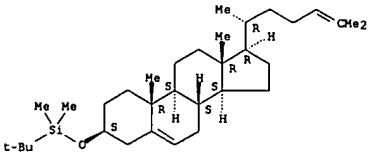
Absolute stereochemistry.

L28 ANSWER 5 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 220150-72-1 CAPLUS
CN Silane, [(3.beta.)-cholesta-5,24-dien-3-yloxy](1,1-dimethylethyl)dimethyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

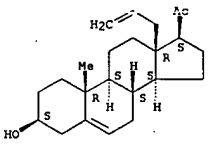
L28 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:737266 CAPLUS
DOCUMENT NUMBER: 130:95713
TITLE: 18-Vinyldeoxycorticosterone: a potent inhibitor of the bovine cytochrome P-45011.beta.
AUTHOR(S): Davioud, Elisabeth; Piffeteau, Annie; Delorme, Cecile; Coustal, Suzy; Marquet, Andree
CORPORATE SOURCE: Laboratoire de Chimie Organique Biologique, Universite Pierre et Marie Curie, CNRS UMR 7613, Paris, 75252, Fr.
SOURCE: Bioorganic & Medicinal Chemistry (1998), 6(10), 1781-1788
CODEN: BMECEP; ISSN: 0968-0896
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 18-Vinylprogesterone (18-VP) and 18-ethynylprogesterone (18-EP) have proved to be potent suicide inhibitors of P 45011.beta., the last enzyme of aldosterone biosynthesis (Delorme, C.; Piffeteau, A.; Viger, A.; Marquet, A. Eur. J. Biochem. 1995, 232, 247; Delorme, C.; Piffeteau, A.; Sobrio, F.; Marquet, A. Eur. J. Biochem. 1997, 248, 252). This paper describes the synthesis of 18-vinyldeoxycorticosterone (18-VDOC), an analog of deoxycorticosterone (DOC), the physiol. substrate of the enzyme, and the evaluation of its reversible inhibiting properties for deoxycorticosterone and corticosterone oxidn. by the bovine enzyme. 18-VDOC has been obtained by hydroxylation at C-21 of a 18-VP precursor. Its reversible Ki values are, resp., 0.3 .mu.M for the 11.beta.-hydroxylation and 0.8 .mu.M for the 18-hydroxylation. Hence, 18-VDOC is the strongest competitive inhibitor of bovine P 45011.beta. described so far, but in contrast with 18-VP, it does not inhibit more efficiently the 18-hydroxylation than the 11-hydroxylation.

IT **219120-06-6P 219120-07-7P 219120-08-8P 219120-09-9P 219120-10-2P 219120-12-4P 219120-14-6P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and biol. activity of 18-vinyldeoxycorticosterone as a potent inhibitor of the bovine cytochrome P 45011.beta.)

RN 219120-06-6 CAPLUS
CN 18-Norpregn-5-en-20-one, 3-hydroxy-13-(2-propenyl)-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

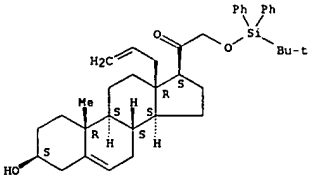


RN 219120-07-7 CAPLUS

L28 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

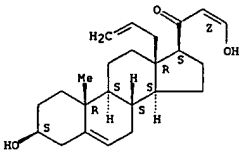
RN 219120-10-2 CAPLUS
CN 18-Norpregn-5-en-20-one, 21-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-3-hydroxy-13-(2-propenyl)-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 219120-12-4 CAPLUS
CN 2-Propen-1-one, 3-hydroxy-1-[(3.beta.,17.beta.)-3-hydroxy-13-(2-propenyl)-18-norandrost-5-en-17-yl]-, (2Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.

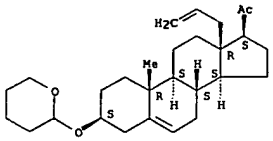


RN 219120-14-6 CAPLUS
CN Silane, trimethyl[[(3.beta.)-13-(2-propenyl)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-18-norpregna-5,20-dien-20-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

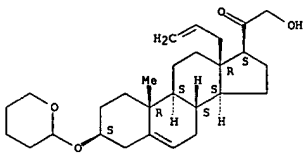
L28 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
CN 18-Norpregn-5-en-20-one, 13-(2-propenyl)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



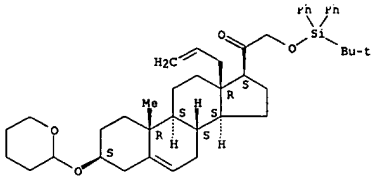
RN 219120-08-8 CAPLUS
CN 18-Norpregn-5-en-20-one, 21-hydroxy-13-(2-propenyl)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

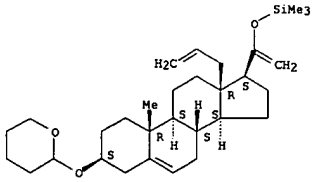


RN 219120-09-9 CAPLUS
CN 18-Norpregn-5-en-20-one, 21-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-13-(2-propenyl)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



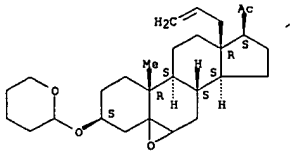
L28 ANSWER 6 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT **219143-68-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(synthesis and biol. activity of 18-vinyldeoxycorticosterone as a potent inhibitor of the bovine cytochrome P 45011.beta.)

RN 219143-68-7 CAPLUS
CN 18-Norpregnan-20-one, 5,6-epoxy-13-(2-propenyl)-3-[(tetrahydro-2H-pyran-2-yl)oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

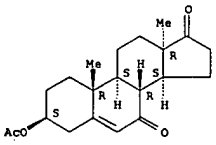
Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 7 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:725635 CAPLUS
DOCUMENT NUMBER: 130:66658
TITLE: The preparation of some 13.alpha.-androstanes
AUTHOR(S): Hanson, James R.; Hunter, A. Christy; Roquier, Sandrine
CORPORATE SOURCE: School of Chemistry, Physics and Environmental Science, University of Sussex, Sussex, BN1 9QJ, UK
SOURCE: Collection of Czechoslovak Chemical Communications (1998), 63(10), 1646-1654
CODEN: CCCCAK; ISSN: 0010-0765
PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:66658
AB The prepn. of 17a-oxa-17a-homo-5.alpha.,13.alpha.-androstane-3,17-dione (I), 5.alpha.,13.alpha.-androstane-3,7,17-trione (II), 4-chloro- (III; R = Cl) and 4-hydroxy-13.alpha.-androst-4-ene-3,17-dione (III; R = OH) and 13.alpha.-androst-4-ene-3,6,17-trione (IV) is described.
IT **218140-93-3P**, 3.beta.-Acetoxy-13.alpha.-androst-5-ene-7,17-dione **218141-01-6P**, 5.alpha.,6.alpha.-Epoxy-3.beta.-hydroxy-13.alpha.-androstan-17-one
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of some 13.alpha.-androstanes)
RN 218140-93-3 CAPLUS
CN Androst-5-ene-7,17-dione, 3-(acetyloxy)-, (3.beta.,13.alpha.)- (9CI) (CA INDEX NAME)

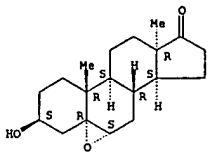
Absolute stereochemistry.



RN 218141-01-6 CAPLUS
CN Androstan-17-one, 5,6-epoxy-3-hydroxy-, (3.beta.,5.alpha.,6.alpha.,13.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

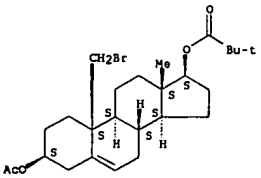
L28 ANSWER 7 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 8 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:725631 CAPLUS
DOCUMENT NUMBER: 130:81693
TITLE: Synthesis and photochemical transformations of 19-phenylsulfonyl provitamin D analog
AUTHOR(S): Grzegorzewski, Piotr; Koladkiewicz, Izabela; Morzycki, Jacek W.; Sicinski, Rafal R.
CORPORATE SOURCE: Department of Chemistry, University of Warsaw, Warsaw, 02-093, Pol.
SOURCE: Collection of Czechoslovak Chemical Communications (1998), 63(10), 1597-1612
CODEN: CCCCAK; ISSN: 0010-0765
PUBLISHER: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 130:81693
AB The synthesis of provitamin D analog 19-(phenylsulfonyl)androsta-5,7-diene-3.beta.,17.beta.-diyl 3-acetate 17-pivalate (I) has been accomplished from 19-hydroxyandrost-5-ene-3.beta.,17.beta.-diyl 3-acetate 17-pivalate (II). II was first obtained in low yield in the nucleophilic displacement reactions of 19-halogenated-5-ene steroids with sodium benzenesulfinate. Then a more efficient method has been used, which involves protection of the double bond as an epoxide. Introduction of the C(7)-C(8) double bond into olefin II has also been achieved in two ways. The first involved bromination-dehydrobromination and the other consisted of an allylic oxidn. of olefin II leading to enone and the Bamford-Stevens reaction of its tosylhydrazone. UV irradn. of 5,7-diene I resulted in formation of a complex mixt. of products. The structures of five isolated compds. were established on the basis of their 1H NMR spectra and mechanistic rationale.
IT **218900-37-9P 218900-57-3P 218900-58-4P 218900-60-8P 218900-62-0P 218900-63-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis and photochem. transformations of 19-phenylsulfonyl provitamin D analog)
RN 218900-37-9 CAPLUS
CN Androst-5-ene-3,17-diol, 19-bromo-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,17.beta.)- (9CI) (CA INDEX NAME)

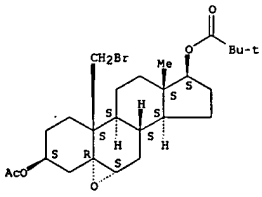
Absolute stereochemistry. Rotation (-).



RN 218900-57-3 CAPLUS
CN Androstane-3,17-diol, 19-bromo-5,6-epoxy-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,5.alpha.,6.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

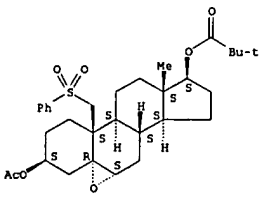
L28 ANSWER 8 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry. Rotation (-).



RN 218900-58-4 CAPLUS
CN Androstane-3,17-diol, 5,6-epoxy-19-(phenylsulfonyl)-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,5.alpha.,6.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

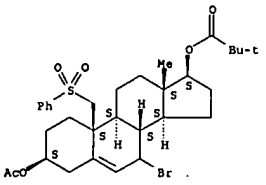
Absolute stereochemistry. Rotation (-).



RN 218900-60-8 CAPLUS
CN Androst-5-ene-3,17-diol, 6-bromo-19-(phenylsulfonyl)-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,17.beta.)- (9CI) (CA INDEX NAME)

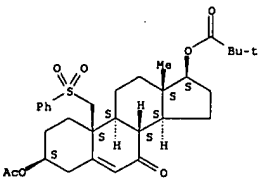
Absolute stereochemistry.

L28 ANSWER 8 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 218900-62-0 CAPLUS
CN Androst-5-en-7-one, 3-(acetyloxy)-17-(2,2-dimethyl-1-oxopropoxy)-19-(phenylsulfonyl)-, (3.beta.,17.beta.)- (9CI) (CA INDEX NAME)

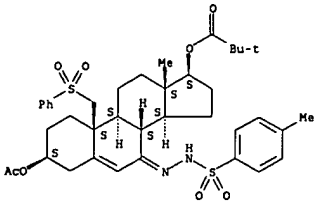
Absolute stereochemistry. Rotation (-).



RN 218900-63-1 CAPLUS
CN Propanoic acid, 2,2-dimethyl-, (3.beta.,17.beta.)-3-(acetyloxy)-7-[[(4-methylphenyl)sulfonyl]hydrazono]-19-(phenylsulfonyl)androst-5-en-17-yl ester (9CI) (CA INDEX NAME)

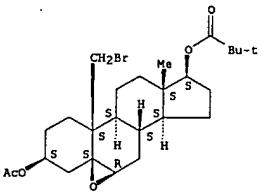
Absolute stereochemistry.
Double bond geometry unknown.

L28 ANSWER 8 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT 218900-59-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis and photochem. transformations of 19-phenylsulfonyl provitamin D analog)
RN 218900-59-5 CAPLUS
CN Androstane-3,17-diol, 19-bromo-5,6-epoxy-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,5.beta.,6.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

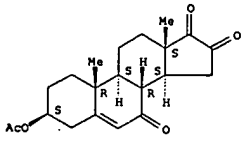
L28 ANSWER 9 OF 38 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER:	1998:663745 CAPLUS
DOCUMENT NUMBER:	130:25222
TITLE:	Ergosteroids III. Syntheses and biological activity of seco-steroids related to dehydroepiandrosterone
AUTHOR(S):	Reich, Ieva L.; Lardy, Henry; Wei, Yong; Marwah, Padma; Kneer, Nancy; Powell, Douglas R.; Reich, Hans J.
CORPORATE SOURCE:	Institute for Enzyme Research and Department of Chemistry, University of Wisconsin-Madison, Madison, WI, 53705, USA
SOURCE:	Steroids (1998), 63(10), 542-553 CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER:	Elsevier Science Inc.
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB The unusual activity of some D-ring-seco estrogens led us to prep. several seco steroids related to dehydroepiandrosterone (DHEA) and to test for their ability to mimic thyroid hormone and 7-oxo-DHEA as inducers of thermogenic enzymes in rats' livers. Only one, 3.beta.-acetoxy-17a-oxa-androst-5-ene-7,17-dione, was capable of inducing both mitochondrial glycerophosphate dehydrogenase and malic enzyme. The closely related 3.beta.-hydroxy-17a-oxa-androsta-5,15-diene-7,17-diones induce the formation of malic enzyme but not of glycerophosphate dehydrogenase. The 3.beta.-propionyl ester of the above 14.alpha. steroid was not active, presumably because it was not deacylated in vivo. The 16,17 dicarboxylic acid produced by opening the D-ring also induced the formation of malic enzyme but not of glycerophosphate dehydrogenase. 3.beta.-Acetoxyandrost-5-ene-7,16,17-trione, an intermediate in the synthesis of D-ring seco compds. enhanced the formation of both enzymes. Twelve other D-ring seco compds. were not active. Seco androstanes oxygenated at position 7 and with expanded A or B rings were not active.

IT 165181-86-2P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of secosteroids related to dehydroepiandrosterone as inducers of thermogenic enzymes)
RN 165181-86-2 CAPLUS
CN Androst-5-ene-7,16,17-trione, 3-(acetyloxy)-, (3.beta.)- (9CI) (CA INDEX NAME)

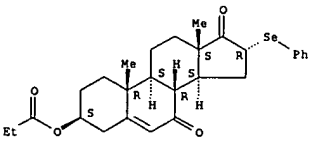
Absolute stereochemistry.



IT 216485-15-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(synthesis of secosteroids related to dehydroepiandrosterone as inducers of thermogenic enzymes)

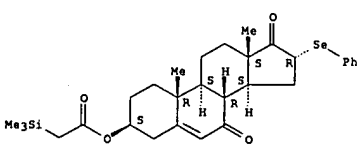
L28 ANSWER 9 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
RN 216485-15-3 CAPLUS
CN Androst-5-ene-7,17-dione, 3-(1-oxopropoxy)-16-(phenylseleno)-, (3.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



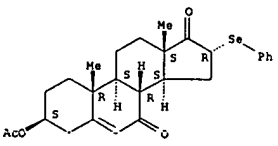
IT 216484-81-0P 216484-82-1P 216484-83-2P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of secosteroids related to dehydroepiandrosterone as inducers of thermogenic enzymes)
RN 216484-81-0 CAPLUS
CN Androst-5-ene-7,17-dione, 16-(phenylseleno)-3-[[(trimethylsilyl)acetyl]oxy]-, (3.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



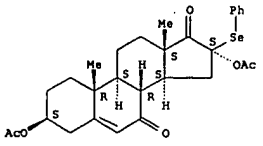
RN 216484-82-1 CAPLUS
CN Androst-5-ene-7,17-dione, 3-(acetyloxy)-16-(phenylseleno)-, (3.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



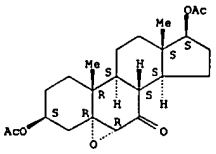
L28 ANSWER 9 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
RN 216484-83-2 CAPLUS
CN Androst-5-ene-7,17-dione, 3,16-bis(acetyloxy)-16-(phenylseleno)-, (3.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **64936-63-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(synthesis of secosteroids related to dehydroepiandrosterone as inducers of thermogenic enzymes)
RN 64936-63-6 CAPLUS
CN Androstan-7-one, 3,17-bis(acetyloxy)-5,6-epoxy-, (3.beta.,5.alpha.,6.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

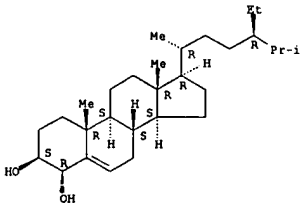
Absolute stereochemistry.



REFERENCE COUNT: 29 THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L28 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:185142 CAPLUS
DOCUMENT NUMBER: 128:230561
TITLE: Modified sterols. XIV. Synthesis of 3.beta.,4.beta.-dihydroxy-6-ketosterols from the phytosterols .beta.-campesterol and .beta.-sitosterol
AUTHOR(S): Irismetov, M. P.; Dzhiembaev, B. Zh.; Verlinskaya, L. V.; Praliev, K. D.
CORPORATE SOURCE: Inst. Khim. Nauk im. Bekturova, Almaty, Kazakhstan
SOURCE: Izvestiya Ministerstva Nauki--Akademii Nauk Respubliki Kazakhstan, Seriya Khimicheskaya (1997), (3), 50-54
CODEN: IMKKFL
PUBLISHER: Gylym
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 128:230561
AB Allylic hydroxylation of the phytosterols .beta.-campesterol (I; R = Me) and .beta.-sitosterol (I; R = Et) with selenium dioxide was studied. 3.beta.,4.beta.-Dihydroxy-6-ketosterols of .beta.-campesterol and .beta.-sitosterol were synthesized.
IT **141602-53-1P 141602-54-2P 141602-55-3P 204765-57-1P 204765-59-3P 204765-60-6P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of 3.beta.,4.beta.-dihydroxy-6-ketosterols from .beta.-campesterol and .beta.-sitosterol)
RN 141602-53-1 CAPLUS
CN Stigmast-5-ene-3,4-diol, (3.beta.,4.beta.)- (9CI) (CA INDEX NAME)

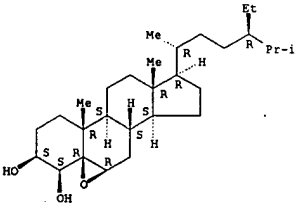
Absolute stereochemistry.



RN 141602-54-2 CAPLUS
CN Stigmastane-3,4-diol, 5,6-epoxy-, (3.beta.,4.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

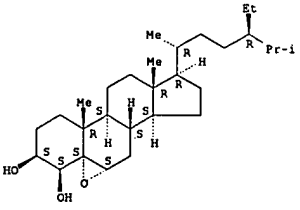
Absolute stereochemistry.

L28 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



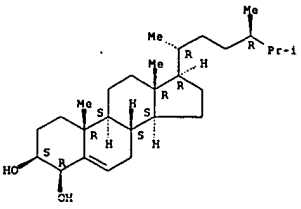
RN 141602-55-3 CAPLUS
CN Stigmastane-3,4-diol, 5,6-epoxy-, (3.beta.,4.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204765-57-1 CAPLUS
CN Ergost-5-ene-3,4-diol, (3.beta.,4.beta.,24R)- (9CI) (CA INDEX NAME)

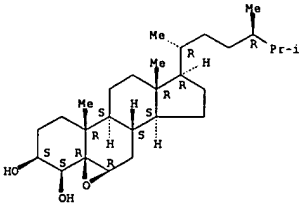
Absolute stereochemistry.



L28 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

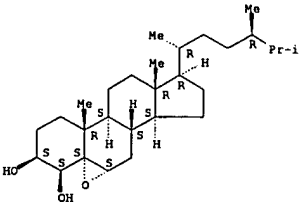
RN 204765-59-3 CAPLUS
CN Ergostane-3,4-diol, 5,6-epoxy-, (3.beta.,4.beta.,5.beta.,6.beta.,24R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204765-60-6 CAPLUS
CN Ergostane-3,4-diol, 5,6-epoxy-, (3.beta.,4.beta.,5.alpha.,6.alpha.,24R)- (9CI) (CA INDEX NAME)

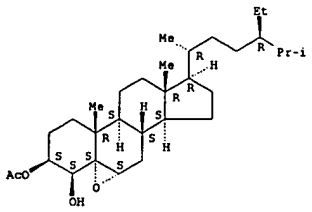
Absolute stereochemistry.



IT **141602-56-4P 204765-62-8P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of 3.beta.,4.beta.-dihydroxy-6-ketosterols from .beta.-campesterol and .beta.-sitosterol)
RN 141602-56-4 CAPLUS
CN Stigmastane-3,4-diol, 5,6-epoxy-, 3-acetate, (3.beta.,4.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

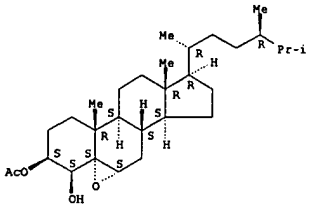
Absolute stereochemistry.

L28 ANSWER 10 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 204765-62-8 CAPLUS
CN Ergostane-3,4-diol, 5,6-epoxy-, 3-acetate, (3.beta.,4.beta.,5.alpha.,6.alpha.,24R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



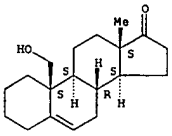
L28 ANSWER 11 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:129375 CAPLUS
DOCUMENT NUMBER: 128:217536
TITLE: Reaction of androst-5-en-17-one with hypobromous acid and its use for synthesis of 19-oxygenated 5-ene and 4-en-6-one steroids
AUTHOR(S): Numazawa, Mitsuteru; Yamada, Keiko
CORPORATE SOURCE: Tohoku College of Pharmacy, Sendai, 981, Japan
SOURCE: Steroids (1998), 63(2), 62-69
CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 128:217536

AB Reaction of androst-5-en-17-one with hypobromous acid using a short reaction time (30 min) along with a careful isolation procedure gave, for the first time, the addn. product, 5.alpha.-bromo-6.beta.-hydroxyandrostan-17-one (I), in 43% yield. This bromohydrin was much more reactive than 5.alpha.-bromo-3.beta.-acetoxy-6.beta.-hydroxyandrostan-17-one towards KHCO3 and HClO4. The high reactivity of compd. I was found to be a principal reason for the difficulty in isolating this compd. by the addn. reaction so far. 19-Hydroxyandrost-5-en-17-one and androst-5-ene-17,19-dione, as well as 19-hydroxyandrost-4-ene-6,17-dione and androst-4-ene-6,17,19-trione, were synthesized through hypoiodite reaction of the bromohydrin I as a key reaction.

IT **157022-95-2P 204330-82-5P 204330-89-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(reaction of androst-5-en-17-one with hypobromous acid and use for synthesis of 19-oxygenated 5-ene and 4-en-6-one steroids)

RN 157022-95-2 CAPLUS
CN Androst-5-en-17-one, 19-hydroxy- (9CI) (CA INDEX NAME)

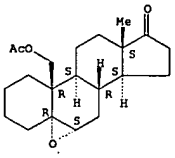
Absolute stereochemistry.



RN 204330-82-5 CAPLUS
CN Androstan-17-one, 19-(acetyloxy)-5,6-epoxy-, (5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

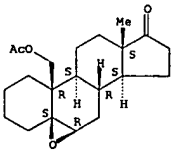
Absolute stereochemistry.

L28 ANSWER 11 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 204330-89-2 CAPLUS
CN Androstan-17-one, 19-(acetyloxy)-5,6-epoxy-, (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

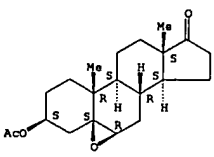
Absolute stereochemistry.



IT **6585-68-8P 117926-18-8P 131768-89-3P**
204330-81-4P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(reaction of androst-5-en-17-one with hypobromous acid and use for synthesis of 19-oxygenated 5-ene and 4-en-6-one steroids)

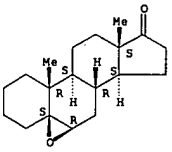
RN 6585-68-8 CAPLUS
CN Androstan-17-one, 3-(acetyloxy)-5,6-epoxy-, (3.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



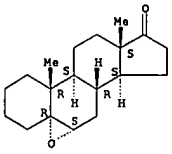
RN 117926-18-8 CAPLUS
CN Androstan-17-one, 5,6-epoxy-, (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

L28 ANSWER 11 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
Absolute stereochemistry.



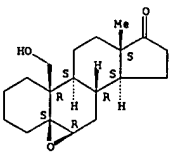
RN 131768-89-3 CAPLUS
CN Androstan-17-one, 5,6-epoxy-, (5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 204330-81-4 CAPLUS
CN Androstan-17-one, 5,6-epoxy-19-hydroxy-, (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

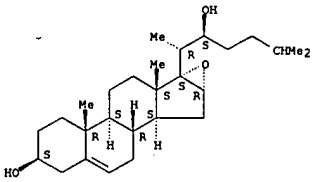
L28 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1998:120410 CAPLUS
DOCUMENT NUMBER: 128:205029
TITLE: Cephalostatin support studies. 12. The first synthesis of the aglycon of the potent anti-tumor steroidal saponin OSW-1
AUTHOR(S): Guo, Chuangxing; Fuchs, P. L.
CORPORATE SOURCE: Dep. Chem., Purdue Univ., West Lafayette, IN, 47907, USA
SOURCE: Tetrahedron Letters (1998), 39(10), 1099-1102
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The protected aglycon (I) of the potent antitumor agent OSW-1 was synthesized in 9 steps from 5-androsten-3.beta.-ol-17-one in 55% overall yield. Key reactions involve ene installation of the side chain, regio and stereoselective dihydroxylation and diastereoselective redn. of the C16 ketone.

IT **203987-05-7P 203987-14-8P 203987-16-0P**
203987-19-3P 203987-25-1P 203987-30-8P
203987-33-1P 203987-34-2P 203987-35-3P
203987-36-4P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis of aglycon of steroidal saponin OSW-1)

RN 203987-05-7 CAPLUS
CN Cholest-5-ene-3,22-diol, 16,17-epoxy-, (3.beta.,16.alpha.,22S)- (9CI) (CA INDEX NAME)

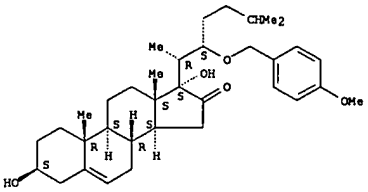
Absolute stereochemistry.



RN 203987-14-8 CAPLUS
CN Cholest-5-en-16-one, 3,17-dihydroxy-22-[(4-methoxyphenyl)methoxy]-, (3.beta.,22S)- (9CI) (CA INDEX NAME)

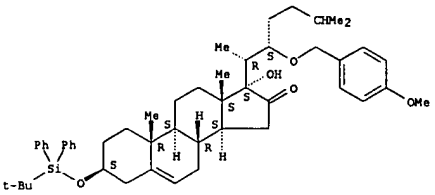
Absolute stereochemistry.

L28 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 203987-16-0 CAPLUS
CN Cholest-5-en-16-one, 3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-17-hydroxy-22-[(4-methoxyphenyl)methoxy]-, (3.beta.,22S)- (9CI) (CA INDEX NAME)

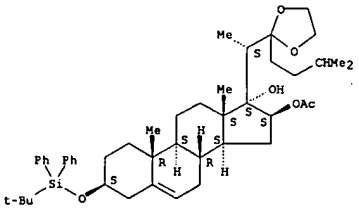
Absolute stereochemistry.



RN 203987-19-3 CAPLUS
CN Cholest-5-en-22-one, 16-(acetyloxy)-3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-17-hydroxy-, cyclic 22-(1,2-ethanediyl acetal), (3.beta.,16.beta.)- (9CI) (CA INDEX NAME)

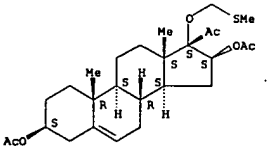
Absolute stereochemistry.

L28 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



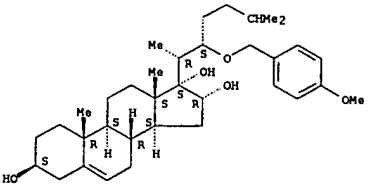
RN 203987-25-1 CAPLUS
CN Pregn-5-en-20-one, 3,16-bis(acetyloxy)-17-[(methylthio)methoxy]-, (3.beta.,16.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 203987-30-8 CAPLUS
CN Cholest-5-ene-3,16,17-triol, 22-[(4-methoxyphenyl)methoxy]-, (3.beta.,16.alpha.,22S)- (9CI) (CA INDEX NAME)

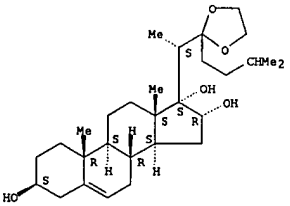
Absolute stereochemistry.



RN 203987-33-1 CAPLUS
CN Cholest-5-en-22-one, 3,16,17-trihydroxy-, cyclic 1,2-ethanediyl acetal, (3.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

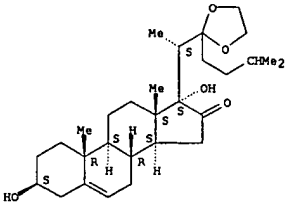
L28 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

Absolute stereochemistry.



RN 203987-34-2 CAPLUS
CN Cholest-5-ene-16,22-dione, 3,17-dihydroxy-, cyclic 22-(1,2-ethanediyl acetal), (3.beta.)- (9CI) (CA INDEX NAME)

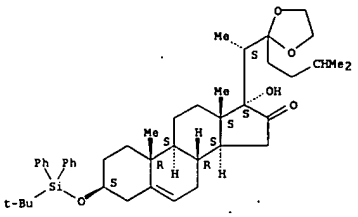
Absolute stereochemistry.



RN 203987-35-3 CAPLUS
CN Cholest-5-ene-16,22-dione, 3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-17-hydroxy-, cyclic 22-(1,2-ethanediyl acetal), (3.beta.)- (9CI) (CA INDEX NAME)

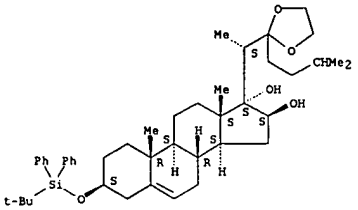
Absolute stereochemistry.

L28 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 203987-36-4 CAPLUS
CN Cholest-5-en-22-one, 3-[[(1,1-dimethylethyl)diphenylsilyl]oxy]-16,17-dihydroxy-, cyclic 1,2-ethanediyl acetal, (3.beta.,16.beta.)- (9CI) (CA INDEX NAME)

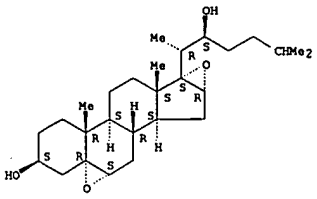
Absolute stereochemistry.



IT 203987-28-4P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of aglycon of steroidal saponin OSW-1)
RN 203987-28-4 CAPLUS
CN Cholestane-3,22-diol, 5,6:16,17-diepoxy-, (3.beta.,5.alpha.,6.alpha.,16.alpha.,22S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L28 ANSWER 12 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



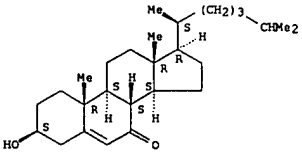
L28 ANSWER 13 OF 38 CAPLUS COPYRIGHT 2003 ACS

ACCESSION NUMBER: 1998:39823 CAPLUS
DOCUMENT NUMBER: 128:114551
TITLE: A convenient acylation procedure for alcohols and amines
AUTHOR(S): Misharin, A. Yu.; Chernov, B. K.
CORPORATE SOURCE: Institute Experimental Cardiology, Cardiological Research Center, Russian Academy Medical Sciences, Moscow, 121552, Russia
SOURCE: Bioorganicheskaya Khimiya (1997), 23(8), 675-679
CODEN: BIKHD7; ISSN: 0132-3423
PUBLISHER: MAIK Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The reaction of carboxylic acids with primary and secondary alcs. in the presence of mesitylenesulfonyl chloride, 2,4,6-triisopropylbenzenesulfonyl chloride, mesitylenesulfonyl tetrazolide, or 2,4,6-triisopropylbenzenesulfonyl tetrazolide and typical acylation catalysts was shown to be a convenient procedure for the synthesis of esters. Reaction of carboxylic acids with primary aliph. or arom. amines in the presence of the same tetrazolides and catalysts was a useful procedure for the synthesis of amides. Syntheses of 20 compds. are presented as examples.

IT 201731-16-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(acylation of alcs. and amines in presence of arenesulfonyl chlorides or (arenesulfonyl)tetrazoles)
RN 201731-16-0 CAPLUS
CN Cholest-5-en-7-one, 3-hydroxy-, (3.beta.,20S)- (9CI) (CA INDEX NAME)

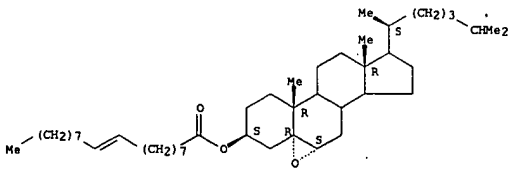
Absolute stereochemistry.



IT 201412-85-3P 201731-21-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(acylation of alcs. and amines in presence of arenesulfonyl chlorides or (arenesulfonyl)tetrazoles)
RN 201412-85-3 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, 9-octadecenoate, (3.beta.,5.alpha.,6.alpha.,8.xi.,9.xi.,14.xi.,17.xi.,20S)- (9CI) (CA INDEX NAME)

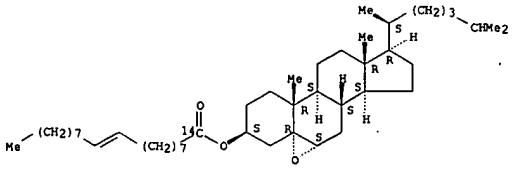
Absolute stereochemistry.
Double bond geometry unknown.

L28 ANSWER 13 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

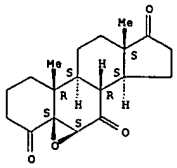


RN 201731-21-7 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, 9-octadecenoate-1-14C, (3.beta.,5.alpha.,6.alpha.,20S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

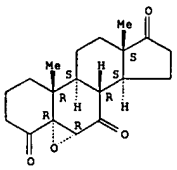


L28 ANSWER 15 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
Absolute stereochemistry.



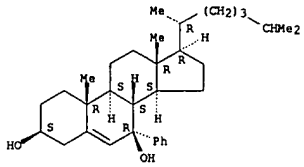
RN 191806-69-6 CAPLUS
CN Androstane-4,7,17-trione, 5,6-epoxy-, (5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:266870 CAPLUS
DOCUMENT NUMBER: 126:293491
TITLE: Unusual oxidation reactions of 7.alpha.-methyl- and 7.alpha.-phenylcholest-5-ene-3.beta.,7.beta.-diol
AUTHOR(S): Morzycki, J. W.; Dabrowski, Z.; Trusewicz, M.; Wilczewska, A. Z.
CORPORATE SOURCE: Inst. Chemistry, Univ. Warsaw, Bialystok, 15443, Pol.
SOURCE: Monatshefte fuer Chemie (1996), 127(12), 1283-1289
CODEN: MOCMB7; ISSN: 0026-9247
PUBLISHER: Springer
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 126:293491
AB Ozonization of 7.alpha.-methyl- or 7.alpha.-phenylcholest-5-ene-3.beta.,7.beta.-diol 3-TBDMS ether (TBDMS = Me3CMe2Si) afforded the corresponding 5.beta.,6.beta.-epoxides. The same product was formed by MCPBA oxidn. The reaction of 7.alpha.-phenylcholest-5-ene-3.beta.,7.beta.-diol with CrO3 yielded 3,7-dioxo-6,7-seco-7-phenylcholest-4-ene-5-carboxaldehyde. An analogous B-seco aldehyde was obtained from 7.alpha.-methylcholest-5-ene-3.beta.,7.beta.-diol in addn. to 7-methylcholesta-4,6-dien-3-one. Jones oxidn. of 7.alpha.-phenylcholest-5-ene-3.beta.,7.beta.-diol or B-seco-aldehyde gave 3,7-dioxo-6,7-seco-7-phenylcholest-4-en-6-oate isolated as its Me ester upon treatment with CH2N2.
IT **149280-66-0 149280-68-2**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(oxidn. of methyl- and phenylcholestenediol)
RN 149280-66-0 CAPLUS
CN Cholest-5-ene-3,7-diol, 7-phenyl-, (3.beta.,7.beta.)- (9CI) (CA INDEX NAME)

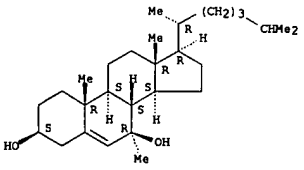
Absolute stereochemistry.



RN 149280-68-2 CAPLUS
CN Cholest-5-ene-3,7-diol, 7-methyl-, (3.beta.,7.beta.)- (9CI) (CA INDEX NAME)

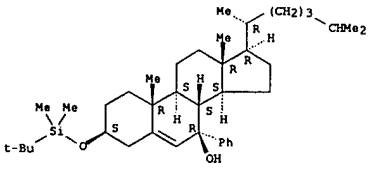
Absolute stereochemistry.

L28 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



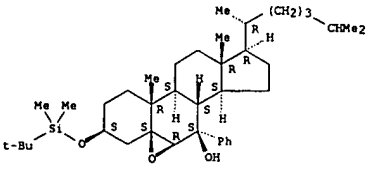
IT **189103-23-9P 189103-26-2P 189103-31-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(oxidn. of methyl- and phenylcholestenediol)
RN 189103-23-9 CAPLUS
CN Cholest-5-en-7-ol, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-phenyl-, (3.beta.,7.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 189103-26-2 CAPLUS
CN Cholestan-7-ol, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,6-epoxy-7-phenyl-, (3.beta.,5.beta.,6.beta.,7.beta.)- (9CI) (CA INDEX NAME)

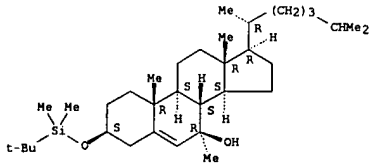
Absolute stereochemistry.



RN 189103-31-9 CAPLUS
CN Cholest-5-en-7-ol, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-7-methyl-,

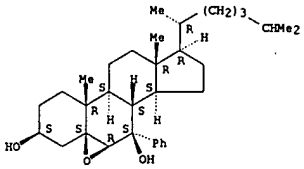
L28 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
(3.beta.,7.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



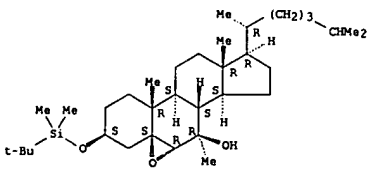
IT **189103-24-0P 189103-25-1P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(oxidn. of methyl- and phenylcholestenediol)
RN 189103-24-0 CAPLUS
CN Cholestane-3,7-diol, 5,6-epoxy-7-phenyl-, (3.beta.,5.beta.,6.beta.,7.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 189103-25-1 CAPLUS
CN Cholestan-7-ol, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-5,6-epoxy-7-methyl-, (3.beta.,5.beta.,6.beta.,7.beta.)- (9CI) (CA INDEX NAME)

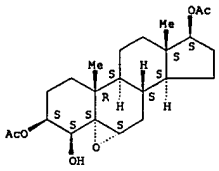
Absolute stereochemistry.



L28 ANSWER 16 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

L28 ANSWER 17 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1997:165734 CAPLUS
DOCUMENT NUMBER: 126:171767
TITLE: The synthesis of N-aryl androsterone pyrazoles as aromatase inhibitors
AUTHOR(S): Li, Shengrong; Parish, Edward J.; Webbe, Thomas; Brodie, Angela M. H.
CORPORATE SOURCE: Dep. Chem., Auburn Univ., Auburn, AL, 36849, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(4), 403-408
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB N-aryl androsterone pyrazoles I and II (R = H, CH2CH:CHPh, CH2Ph, CH2C6H4NO2-4), showing a good inhibitory activity against aromatase, were synthesized. I [R = H (IC50 = 236 nM); R = CH2Ph (IC50 = 342 nM)] and II [R = CH2Ph (IC50 = 245 nM)] were as active as 4-hydroxyandrost-4-ene-3,17-dione (IC50 = 370 nM) as inhibitors of aromatase.
IT **187344-50-9P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of N-aryl androsterone pyrazoles as aromatase inhibitors)
RN 187344-50-9 CAPLUS
CN Androstane-3,4,17-triol, 5,6-epoxy-, 3,17-diacetate, (3.beta.,4.beta.,5.alpha.,6.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

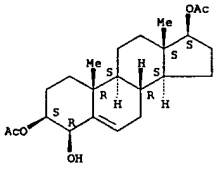
Absolute stereochemistry.



IT **187344-48-5P 187344-49-6P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. of N-aryl androsterone pyrazoles as aromatase inhibitors)
RN 187344-48-5 CAPLUS
CN Androst-5-ene-3,4,17-triol, 3,17-diacetate, (3.beta.,4.beta.,17.beta.)- (9CI) (CA INDEX NAME)

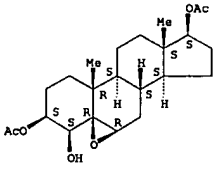
Absolute stereochemistry.

L28 ANSWER 17 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



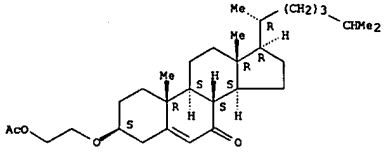
RN 187344-49-6 CAPLUS
CN Androstane-3,4,17-triol, 5,6-epoxy-, 3,17-diacetate, (3.beta.,4.beta.,5.beta.,6.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 18 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1996:752281 CAPLUS
DOCUMENT NUMBER: 126:84406
TITLE: Steryl cellosolves regulate cholesterol metabolism in isolated rabbit hepatocytes
AUTHOR(S): Malyugin, A. V.; Shteinshneider, A. Yu.; Kozykh, V. A.; Alquier, Ch.; Lafont, H.; Misharin, A. Yu.
CORPORATE SOURCE: Inst. Eksper.Kardiol., RAMN, Moscow, 121552, Russia
SOURCE: Bioorganicheskaya Khimiya (1996), 22(8), 606-610
CODEN: BIKHD7; ISSN: 0132-3423
PUBLISHER: MAIK Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB Synthesis of 3.beta.-(2-hydroxyethoxy)cholest-5-ene, 3.beta.-(2-hydroxyethoxy)cholest-5-en-7-one, 3.beta.-(2-hydroxyethoxy)-7.beta.-hydroxycholest-5-ene, 3.beta.-(2-hydroxyethoxy)-5.alpha.,6.beta.-dihydroxycholestane is described. These substances inhibited cholesterol biosynthesis in rabbit hepatocyte cell culture with ID50 from 5.5(.+-.0.7) x 10-8 to 1.3(.+-.0.2) x 10-5 M and also cellular protein biosynthesis.
IT **155252-29-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(intermediate; prepn. of and hepatocyte cholesterol metab. regulation by hydroxyethoxy cholestanes and cholestenes)
RN 155252-29-2 CAPLUS
CN Cholest-5-en-7-one, 3-[2-(acetyloxy)ethoxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

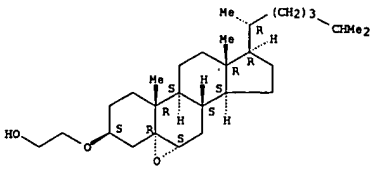
Absolute stereochemistry.



IT **155252-27-0P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(prepn. of and hepatocyte cholesterol metab. regulation by hydroxyethoxy cholestanes and cholestenes)
RN 155252-27-0 CAPLUS
CN Ethanol, 2-[[(3.beta.,5.alpha.,6.alpha.)-5,6-epoxycholestan-3-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L28 ANSWER 18 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



L28 ANSWER 19 OF 38 CAPLUS COPYRIGHT 2003 ACS

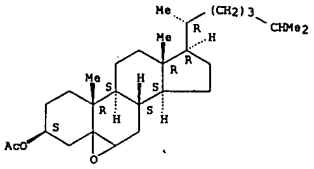
ACCESSION NUMBER: 1996:322182 CAPLUS
DOCUMENT NUMBER: 125:58844
TITLE: A ruthenium-catalyzed oxidation of steroidal alkenes to enones
AUTHOR(S): Miller, Ross A.; Li, Wenjie; Humphrey, Guy R.
CORPORATE SOURCE: Dep. Process Res., Merck Res. Lab., Rahway, NJ, 07065-0900, USA
SOURCE: Tetrahedron Letters (1996), 37(20), 3429-3432
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:58844

AB A new protocol for oxidizing steroidal alkenes to enones has been developed.

IT **55400-50-5P**
RL: BYP (Byproduct); **PREP (Preparation)**
(ruthenium-catalyzed oxidn. of steroidal alkenes to enones)

RN 55400-50-5 CAPLUS
CN Cholestan-3-ol, 5,6-epoxy-, acetate, (3.beta.)- (9CI) (CA INDEX NAME)

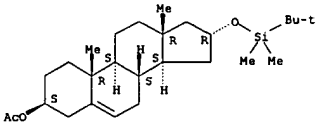
Absolute stereochemistry.



IT **173552-31-3**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(ruthenium-catalyzed oxidn. of steroidal alkenes to enones)

RN 173552-31-3 CAPLUS
CN Androst-5-en-3-ol, 16-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, acetate, (3.beta.,16.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 19 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

L28 ANSWER 20 OF 38 CAPLUS COPYRIGHT 2003 ACS

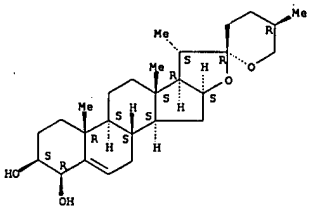
ACCESSION NUMBER: 1996:317703 CAPLUS
DOCUMENT NUMBER: 125:33945
TITLE: Differential behavior of (25R)-5,6-epoxyspirostan-22.alpha.-O-3.beta.-ol and (25R)-5,6-epoxyspirostan-22.alpha.-O-3.beta.,4.beta.-diol toward Dowex
AUTHOR(S): Korde, Shilpa S.; Baig, Mirza H. A.; Desai, Umesh R.; Trivedi, Girish K.
CORPORATE SOURCE: Dep. of Chemistry, Indian Inst. of Technology, Bombay, 400076, India
SOURCE: Steroids (1996), 61(5), 290-295
CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:33945

AB The acid-catalyzed hydrolytic cleavage of the 5,6-epoxyspirostane derivs. by the cation exchange resin Dowex 50W X8 has been exploited with the goal of developing synthetic protocols toward 3,4,5,6-polyhydroxyspirostane analogs that can serve as intermediates to potential biol. active compds. Whereas the diastereomers (25R)-5.alpha.,6.alpha.-epoxyspirostan-22.alpha.-O-3.beta.-ol and (25R)-5.beta.,6.beta.-epoxyspirostan-22.alpha.-O-3.beta.,5.alpha.,6.beta.-triol on Dowex treatment in water-methanol, the .alpha.-and .beta.-diastereomers of the 5,6-epoxy deriv. of 3.beta.,4.beta.-diol provide a single product, (25R)-3.beta.,6.beta.-dihydroxy-5.alpha.-spirostan-4-one, in good yields. The structures of these products have been confirmed using 1H NMR, 13C NMR, and 1H-1H J correlated spectroscopies. Multifunctional product formation suggests tremendous utility of Dowex in steroid synthesis. The product formation has been rationalized on the basis of differential conformational constraints of the A/B rings of the different epoxides in directing the reaction course. The reaction shows an interesting example of stereoelectronic effect of a single hydroxy group in discriminating solvent participation.

IT **177601-42-2**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(differential behavior of (25R)-5,6-epoxyspirostan-22.alpha.-O-3.beta.-ol and (25R)-5,6-epoxyspirostan-22.alpha.-O-3.beta.,4.beta.-diol toward Dowex)

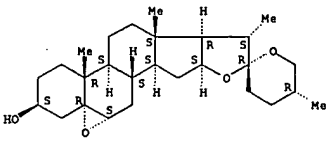
RN 177601-42-2 CAPLUS
CN Spirost-5-ene-3,4-diol, (3.beta.,4.beta.,25R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



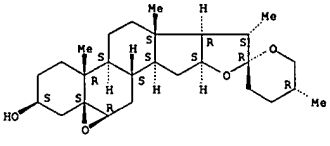
L28 ANSWER 20 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
IT 3514-60-1P 66879-97-8P 177601-43-3P
177601-45-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(differential behavior of (25R)-5,6-epoxyspirostan-22.alpha.-O-3.beta.-ol and (25R)-5,6-epoxyspirostan-22.alpha.-O-3.beta.,4.beta.-diol toward Dowex)
RN 3514-60-1 CAPLUS
CN Spirostan-3-ol, 5,6-epoxy-, (3.beta.,5.alpha.,6.alpha.,25R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 66879-97-8 CAPLUS
CN Spirostan-3-ol, 5,6-epoxy-, (3.beta.,5.beta.,6.beta.,25R)- (9CI) (CA INDEX NAME)

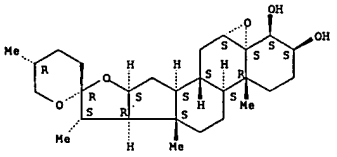
Absolute stereochemistry.



RN 177601-43-3 CAPLUS
CN Spirostan-3,4-diol, 5,6-epoxy-, (3.beta.,4.beta.,5.alpha.,6.alpha.,25R)- (9CI) (CA INDEX NAME)

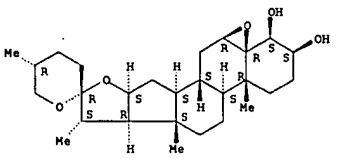
Absolute stereochemistry.

L28 ANSWER 20 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 177601-45-5 CAPLUS
CN Spirostan-3,4-diol, 5,6-epoxy-, (3.beta.,4.beta.,5.beta.,6.beta.,25R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



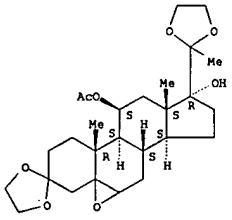
L28 ANSWER 21 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:990826 CAPLUS
DOCUMENT NUMBER: 124:56407
TITLE: Preparation of novel progesterone compound as antitumors, antidiabetics, antirheumatics, and angiostatics
INVENTOR(S): Hibino, Satoshi; Sugino, Eiichi; Kohno, Tetsuya; Fujimori, Shiho; Nemoto, Hideo; Ichihara, Yoshitatsu; Sato, Yoshio
PATENT ASSIGNEE(S): Meiji Milk Products Co., Ltd., Japan
SOURCE: PCT Int. Appl., 25 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9526974	A1	19951012	WO 1995-JP642	19950403
W: JP, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
EP 754701	A1	19970122	EP 1995-913412	19950403
EP 754701	B1	19980812		
R: BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
ES 2119418	T3	19981001	ES 1995-913412	19950403
US 5693629	A	19971202	US 1996-716325	19961004
PRIORITY APPLN. INFO.:			JP 1994-66246	19940404
			WO 1995-JP642	19950403

OTHER SOURCE(S): MARPAT 124:56407
AB Title compds. I [R1 = C1-C23 hydrocarbyl] are prepd. Thus, I [R1 = Me] (II) was prepd. in many steps from 11.beta.,17.alpha.-dihydroxypregn-4-ene-3,20-dione via 11-O-acetylation, 20-acetalization, epoxidn. with m-chloroperbenzoic acid, methylation, hydrolysis, dehydration, fluorination, 3-acetalization, hydrolysis, and 17.alpha.-O-acetylation. In an in vitro study using the chorioallantoic membrane from fertilized eggs, II at 100 .mu.g/egg showed 100% inhibition of angiogenesis vs. 50% inhibition by the known medroxyprogesterone (also at 100 .mu.g/egg).
IT 171611-80-6P 171611-82-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(prepn. of novel progesterone compd. as antitumors, antidiabetics, antirheumatics, and angiostatics)
RN 171611-80-6 CAPLUS
CN Pregnane-3,20-dione, 11-(acetyloxy)-5,6-epoxy-, cyclic 3,20-bis(1,2-ethanediyl acetal), (11.beta.)- (9CI) (CA INDEX NAME)

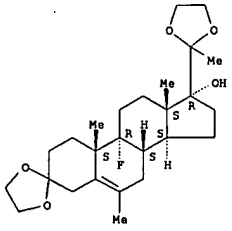
Absolute stereochemistry.

L28 ANSWER 21 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 171611-82-8 CAPLUS
CN Pregn-5-ene-3,20-dione, 9-fluoro-17-hydroxy-6-methyl-, cyclic bis(1,2-ethanediyl acetal) (9CI) (CA INDEX NAME)

Absolute stereochemistry.



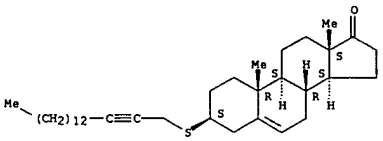
L28 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:836119 CAPLUS
DOCUMENT NUMBER: 123:340531
TITLE: The synthesis and reactivity of 3.beta.-(2-alkynylsulfonyl)- and 3.beta.-(2-alkynylsulfonylmethyl) androst-5-en-17-ones as inhibitors of glucose-6-phosphate dehydrogenase
AUTHOR(S): Williams, John R.; Boehm, Jeffrey C.
CORPORATE SOURCE: Dep. of Chemistry, Temple Univ., Philadelphia, PA, USA
SOURCE: Steroids (1995), 60(10), 699-708
CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB 3.beta.-(Hexadec-2-ynylsulfonyl)androst-5-en-17-one (I, n = 0) was designed as an analog of dehydroepiandrosterone sulfatide, a potent, natural inhibitor of glucose-6-phosphate dehydrogenase (G6PDH). Nucleophilic substitution of 1-bromo hexadec-2-yne with 3.beta.-mercaptoandrost-5-en-17-one followed by oxidn. afforded I (n = 0). The propargylic sulfone I (n = 0) may tautomerize to the electrophilic allenic sulfone and thus function as a masked affinity label of the steroidal binding site of G6PDH. Since I (n = 0) demonstrated low potency as an inhibitor of G6PHD, a sulfonylmethyl analog I (n = 1) was also designed and synthesized. Synthesis of I (n = 1) began by methylenation of androst-5-en-3,17-dione 17-ketal with the Tebbe reagent, to yield the 3-methyleneandrost-5-ene. Hydroboration, followed by oxidn., gave a mixt. of 3.alpha.- and 3.beta.-hydroxymethyl isomers. . The 3.beta. alc. was converted to the thiol followed by alkylation with 1-bromo-2-hexadecyne and selective oxidn. to give the acetylenic sulfone I (n = 1). Insertion of the methylene group significantly increased the G6PDH inhibitory properties over the initial compds.

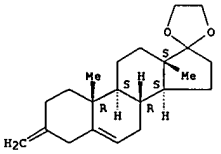
IT **170709-53-2P 170709-54-3P 170709-66-7P**
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); **RCT (Reactant)**; SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and reactivity of 3.beta.-(2-alkynylsulfonyl)- and 3.beta.-(2-alkynylsulfonylmethyl)androst-5-en-17-ones as inhibitors of glucose-6-phosphate dehydrogenase)

RN 170709-53-2 CAPLUS
CN Androst-5-en-17-one, 3-(2-hexadecynylthio)-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

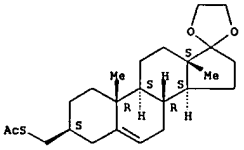


L28 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



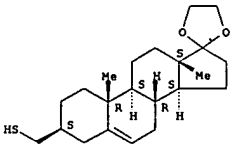
RN 170709-57-6 CAPLUS
CN Androst-5-en-17-one, 3-[(acetylthio)methyl]-, cyclic 17-(1,2-ethanediyl acetal), (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 170709-58-7 CAPLUS
CN Androst-5-en-17-one, 3-(mercaptomethyl)-, cyclic 1,2-ethanediyl acetal, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

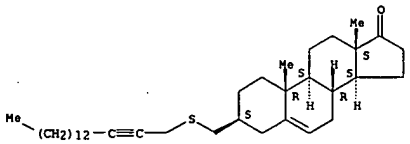


RN 170709-62-3 CAPLUS
CN Androst-5-en-17-one, 3-(bromomethyl)-, cyclic 1,2-ethanediyl acetal, (3.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

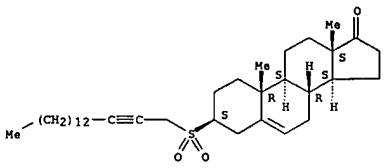
L28 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
RN 170709-54-3 CAPLUS
CN Androst-5-en-17-one, 3-[(2-hexadecynylthio)methyl]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 170709-66-7 CAPLUS
CN Androst-5-en-17-one, 3-(2-hexadecynylsulfonyl)-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

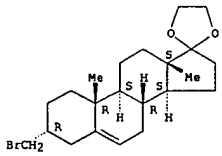


IT **170709-55-4P 170709-57-6P 170709-58-7P**
170709-62-3P 170709-67-8P 170709-69-0P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(synthesis and reactivity of 3.beta.-(2-alkynylsulfonyl)- and 3.beta.-(2-alkynylsulfonylmethyl)androst-5-en-17-ones as inhibitors of glucose-6-phosphate dehydrogenase)

RN 170709-55-4 CAPLUS
CN Androst-5-en-17-one, 3-methylene-, cyclic 1,2-ethanediyl acetal (9CI) (CA INDEX NAME)

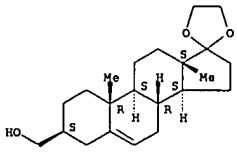
Absolute stereochemistry.

L28 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



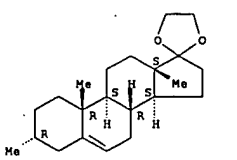
RN 170709-67-8 CAPLUS
CN Androst-5-en-17-one, 3-(hydroxymethyl)-, cyclic 1,2-ethanediyl acetal, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 170709-69-0 CAPLUS
CN Androst-5-en-17-one, 3-methyl-, cyclic 1,2-ethanediyl acetal, (3.alpha.)- (9CI) (CA INDEX NAME)

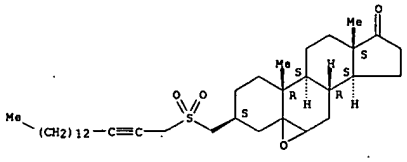
Absolute stereochemistry.



IT **170709-61-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(synthesis and reactivity of 3.beta.-(2-alkynylsulfonyl)- and 3.beta.-(2-alkynylsulfonylmethyl)androst-5-en-17-ones as inhibitors of glucose-6-phosphate dehydrogenase)

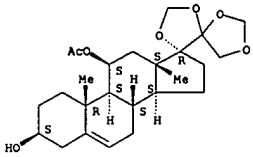
RN 170709-61-2 CAPLUS
CN Androstan-17-one, 5,6-epoxy-3-[(2-hexadecynylsulfonyl)methyl]-, (3.beta.)- (9CI) (CA INDEX NAME)

L28 ANSWER 22 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
Absolute stereochemistry.



L28 ANSWER 23 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:821542 CAPLUS
DOCUMENT NUMBER: 123:286377
TITLE: Synthesis of 19-hydroxysteroids. III. Approaches to the synthesis of 19-hydroxycortisol from cortisol and cortisone
AUTHOR(S): Kovganko, N. V.; Kashkan, Zh. N.; Chernov, Yu. G.
CORPORATE SOURCE: Inst. Bioorg. Khim., Minsk, Belarus
SOURCE: Khimiya Prirodnykh Soedinenii (1993), (3), 374-84
CODEN: KPSUAR; ISSN: 0023-1150
PUBLISHER: Fan
DOCUMENT TYPE: Journal
LANGUAGE: Russian
AB 19-Hydroxycortisol (I) was obtained in multistep syntheses from cortisol and cortisone.
IT **169305-96-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of hydroxycortisol from cortisol and cortisone)
RN 169305-96-8 CAPLUS
CN Pregn-5-ene-3,11-diol, 17,20:20,21-bis[methylenebis(oxy)]-, 11-acetate, (3.beta.,11.beta.)- (9CI) (CA INDEX NAME)

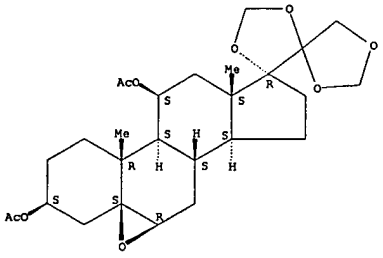
Absolute stereochemistry.



IT **169305-97-9P 169306-06-3P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of hydroxycortisol from cortisol and cortisone)
RN 169305-97-9 CAPLUS
CN Pregnane-3,11-diol, 5,6-epoxy-17,20:20,21-bis[methylenebis(oxy)]-, diacetate, (3.beta.,5.beta.,6.beta.,11.beta.)- (9CI) (CA INDEX NAME)

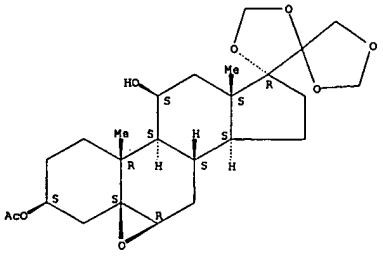
Absolute stereochemistry.

L28 ANSWER 23 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



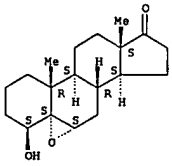
RN 169306-06-3 CAPLUS
CN Pregnane-3,11-diol, 5,6-epoxy-17,20:20,21-bis[methylenebis(oxy)]-, 3-acetate, (3.beta.,5.beta.,6.beta.,11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:745335 CAPLUS
DOCUMENT NUMBER: 123:286372
TITLE: Competing pathway involved in allylic acetoxylation of androst-5-en-17-one and oxidation of allylic alcohols with chromium oxides
AUTHOR(S): Numazawa, Mitsuteru; Tachibana, Mii; Kamiza, Miyako
CORPORATE SOURCE: Tohoku College Pharmacy, Sendai, 981, Japan
SOURCE: Steroids (1995), 60(8), 499-505
CODEN: STEDAM; ISSN: 0039-128X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Allylic acetoxylation of androst-5-en-17-one with Br and Ag(OAc)2 gave 6.alpha.- and 6.beta.-acetoxyandrost-4-en-17-ones (I and II; 3 and 12%, resp.) and 5.alpha.-bromo-6.beta.-acetoxyandrostan-17-one (III; 4%) along with 4.beta.-acetoxyandrost-5-en-17-one (IV; 45%). Treatment of 5.alpha.,6.beta.-dibromoandrostan-17-one, an intermediate of the acetoxylation reaction, with Ag(OAc)2 also produced I-IV in similar relative yields. I and II are produced through a competing pathway involving formation of a bridged carbonium ion followed by attack of AcO-. Oxidn. of 4.beta.-hydroxyandrost-5-en-17-one with Jones reagent did not yield androst-5-ene-4,17-dione (V) but instead gave a 1:4 mixt. of 5.beta.,6.beta.-epoxyandrostan-4-one and 4.beta.,5.beta.-epoxyandrostane-6-one in high yield. In contrast, a 1:4 mixt. of androst-4-ene-6,17-dione and V was obtained upon treatment with CrO3 in pyridine. The oxidn. of 6.beta.-hydroxyandrost-4-ene gave similar results.
IT **131768-95-1P**, Androstan-17-one, 5,6-epoxy-4-hydroxy-, (4.beta.,5.alpha.,6.alpha.)- **169560-43-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(allylic acetoxylation of androstenone and oxidn. of product allylic alcs. with Cr oxides)
RN 131768-95-1 CAPLUS
CN Androstan-17-one, 5,6-epoxy-4-hydroxy-, (4.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

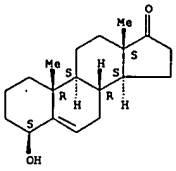
Absolute stereochemistry.



RN 169560-43-4 CAPLUS
CN Androst-5-en-17-one, 4-hydroxy-, (4.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

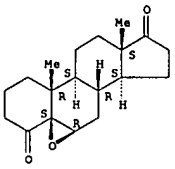
L28 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT **68376-64-7P**, Androstane-4,17-dione, 5,6-epoxy-, (5.beta.,6.beta.)-
117926-18-8P, Androstan-17-one, 5,6-epoxy-, (5.beta.,6.beta.)-
131791-19-0P, Androstan-17-one, 4-(acetyloxy)-5,6-epoxy-, (4.beta.,5.alpha.,6.alpha.)-
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(allylic acetoxylation of androstenone and oxidn. of product allylic alcs. with Cr oxides)

RN 68376-64-7 CAPLUS
CN Androstane-4,17-dione, 5,6-epoxy-, (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

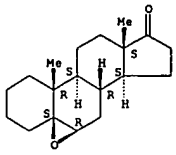
Absolute stereochemistry.



RN 117926-18-8 CAPLUS
CN Androstan-17-one, 5,6-epoxy-, (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

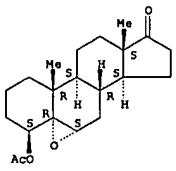
Absolute stereochemistry.

L28 ANSWER 24 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



RN 131791-19-0 CAPLUS
CN Androstan-17-one, 4-(acetyloxy)-5,6-epoxy-, (4.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2003 ACS

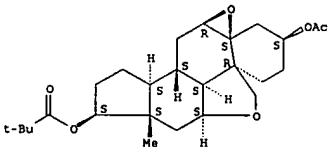
ACCESSION NUMBER: 1995:732942 CAPLUS
DOCUMENT NUMBER: 123:228621
TITLE: Synthesis and photoisomerization of provitamin D analog with 11.beta.,19-oxide bridge
AUTHOR(S): Sicinski, Rafal R.
CORPORATE SOURCE: Dep. Chem., Univ. Warsaw, Warsaw, 02-093, Pol.
SOURCE: Canadian Journal of Chemistry (1995), 73(6), 865-72
CODEN: CJCHAG; ISSN: 0008-4042
PUBLISHER: National Research Council of Canada
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:228621

AB Triol diester I was converted into the B-ring 5,7-diene II representing the first example of the provitamin D analog where the 10.beta. angular Me group is connected to ring C by a C11/C19 ether linkage. UV light irradn. of II resulted in the formation of stereoisomeric 9.beta.,10.alpha.-compd. The structure of the photoproduct was established by anal. of vicinal 1H-1H coupling consts. and by mol. mechanics.

IT **168416-58-8P 168416-59-9P 168416-60-2P**
168416-62-4P 168416-63-5P 168416-64-6P
168416-65-7P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis and photoisomerization of provitamin D analog with 11.beta.,19-oxide bridge)

RN 168416-58-8 CAPLUS
CN Androstane-3,17-diol, 5,6:11,19-diepoxy-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,5.beta.,6.beta.,11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

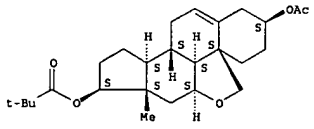
Absolute stereochemistry. Rotation (+).



RN 168416-59-9 CAPLUS
CN Androst-5-ene-3,17-diol, 11,19-epoxy-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

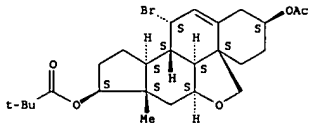
Absolute stereochemistry. Rotation (+).

L28 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



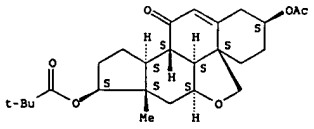
RN 168416-60-2 CAPLUS
CN Androst-5-ene-3,17-diol, 7-bromo-11,19-epoxy-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,7.alpha.,11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 168416-62-4 CAPLUS
CN Androst-5-en-7-one, 3-(acetyloxy)-17-(2,2-dimethyl-1-oxopropoxy)-11,19-epoxy-, (3.beta.,11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

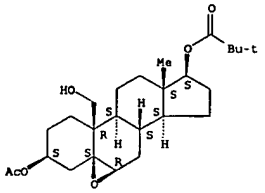
Absolute stereochemistry. Rotation (-).



RN 168416-63-5 CAPLUS
CN Androstane-3,17,19-triol, 5,6-epoxy-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,5.beta.,6.beta.,17.beta.)- (9CI) (CA INDEX NAME)

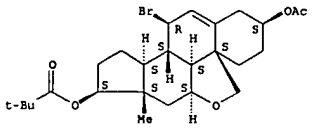
Absolute stereochemistry. Rotation (-).

L28 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



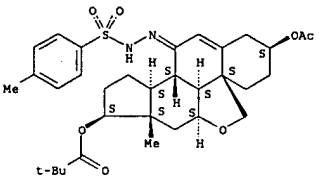
RN 168416-64-6 CAPLUS
CN Androst-5-ene-3,17-diol, 7-bromo-11,19-epoxy-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,7.beta.,11.beta.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 168416-65-7 CAPLUS
CN Benzenesulfonic acid, 4-methyl-, [(3.beta.,11.beta.,17.beta.)-3-(acetyloxy)-17-(2,2-dimethyl-1-oxopropoxy)-11,19-epoxyandrost-5-en-7-ylidene]hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



L28 ANSWER 26 OF 38 CAPLUS COPYRIGHT 2003 ACS

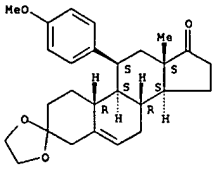
ACCESSION NUMBER: 1995:567321 CAPLUS
DOCUMENT NUMBER: 123:112493
TITLE: Synthesis of 14.beta.-H antiprogestins
AUTHOR(S): Cleve, Arwed; Neef, Guenter; Ottow, Eckhard; Scholz, Stefan; Schwede, Wolfgang
CORPORATE SOURCE: Research Laboratories, Schering AG, Berlin, 13342, Germany
SOURCE: Tetrahedron (1995), 51(19), 5563-72
CODEN: TETRAB; ISSN: 0040-4020
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 123:112493

AB An efficient approach to 14.beta.-H antiprogestins is described. The key step of the synthesis is a cleavage of 17-silyl dienol ethers which are generated from the corresponding .DELTA.14-17-ketones, with hydrogen fluoride-pyridine complex. This method gave access to 14.beta.-H analogs of the 11.beta.,19-bridged series as well as of the 10.beta.-H,11B-aryl series. In both series the inversion at C-14 did not lead to greater sepn. between antiprogestational and antiglucocorticoid activity.

IT **139297-98-6**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(synthesis of 14.beta.-H antiprogestins)

RN 139297-98-6 CAPLUS
CN Estr-5-ene-3,17-dione, 11-(4-methoxyphenyl)-, cyclic 3-(1,2-ethanediyl acetal), (11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **143528-83-0P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(synthesis of 14.beta.-H antiprogestins)

RN 143528-83-0 CAPLUS
CN Estr-15-ene-3,17-dione, 5,6-epoxy-11-(4-methoxyphenyl)-, cyclic 3-(1,2-ethanediyl acetal), (5.alpha.,6.alpha.,11.beta.,14.beta.)- (9CI) (CA INDEX NAME)

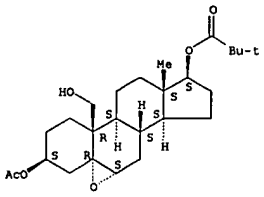
Absolute stereochemistry.

L28 ANSWER 25 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

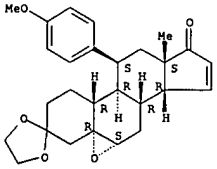
IT **168416-57-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(synthesis and photoisomerization of provitamin D analog with 11.beta.,19-oxide bridge)

RN 168416-57-7 CAPLUS
CN Androstane-3,17,19-triol, 5,6-epoxy-, 3-acetate 17-(2,2-dimethylpropanoate), (3.beta.,5.alpha.,6.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



L28 ANSWER 26 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



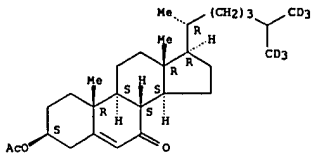
L28 ANSWER 27 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:382256 CAPLUS
DOCUMENT NUMBER: 122:182423
TITLE: Determination of cholesterol oxidation products in human plasma by isotope dilution-mass spectrometry
AUTHOR(S): Dzeletovic, Susanna; Breuer, Olof; Lund, Erik; Diczfalusy, Ulf
CORPORATE SOURCE: Dep. Medical Lab. Sci. Technology, Huddinge Univ. Hospital, Huddinge, S-141 86, Swed.
SOURCE: Analytical Biochemistry (1995), 225(1), 73-80
CODEN: ANBCA2; ISSN: 0003-2697
PUBLISHER: Academic
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A method based on isotope diln.-mass spectrometry was developed for the detn. of nine cholesterol oxidn. products in human plasma. The cholesterol oxidn. products detd. were cholest-5-ene-3.beta.,7.alpha.-diol, cholest-5-ene-3.beta.,7.beta.-diol (7.alpha.- and 7.beta.-hydroxycholesterol, resp.), 3.beta.-hydroxycholest-5-en-7-one (7-oxocholesterol), 5,6.alpha.-epoxy-5.alpha.-cholestan-3.beta.-ol (cholesterol-5.alpha.,6.alpha.-epoxide), 5,6.beta.-epoxy-5.beta.-cholestan-3.beta.-ol (cholesterol-5.beta.,6.beta.-epoxide), cholestane-3.beta.,5.alpha.,6.beta.-triol, cholest-5-ene-3.beta.,24-diol (24-hydroxycholesterol), cholest-5-ene-3.beta.,25-diol (25-hydroxycholesterol), and cholest-5-ene-3.beta.,27-diol (27-hydroxycholesterol). A corresponding deuterium-labeled internal std., contg. 3 to 6 deuterium atoms, was synthesized for each cholesterol oxidn. product except 5.beta.,6.beta.-epoxycholesterol which was detd. using the internal std. for 5.alpha.,6.alpha.-epoxycholesterol. Plasma from 31 healthy volunteers was analyzed by the new method and 27-, 24-, and 7.alpha.-hydroxycholesterol were the most abundant cholesterol oxidn. products (mean values 154, 64, and 43 ng/mL, resp.). The other oxysterols detd. were present in concns. <30 ng/mL. Males had higher 27-hydroxycholesterol concns. in plasma than females. The 5,6-oxygenated products were present mainly unesterified while the other oxidn. products were mostly in esterified form.

IT **161535-78-0**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(detn. of cholesterol oxidn. products in human plasma by isotope-diln. mass spectrometry)
RN 161535-78-0 CAPLUS
CN Cholest-5-en-7-one-26,26,26,27,27,27-d6, 3-(acetyloxy)-, (3.beta.)- (9CI) (CA INDEX NAME)

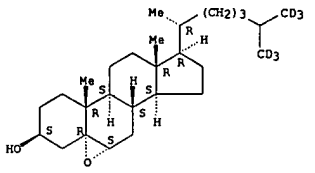
Absolute stereochemistry.

L28 ANSWER 27 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT **161535-75-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(detn. of cholesterol oxidn. products in human plasma by isotope-diln. mass spectrometry)
RN 161535-75-7 CAPLUS
CN Cholestan-26,26,26,27,27,27-d6-3-ol, 5,6-epoxy-, (3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1995:354838 CAPLUS
DOCUMENT NUMBER: 122:178375
TITLE: Steroids and tumor promoter inhibitors containing the steroids
INVENTOR(S): Shudo, Koichi; Endo, Yasuyuki; Hashimoto, Juichi
PATENT ASSIGNEE(S): Shudo Koichi, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

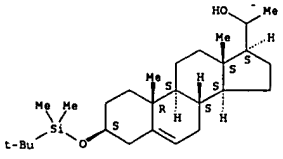
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 06321782	A2	19941122	JP 1993-112760	19930514

PRIORITY APPLN. INFO.: JP 1993-112760 19930514

AB Steroids I [X = :O, OH; R = O2CR1, CHR2R3; R1 = linear or branched alkyl, linear or branched alkenyl, linear or branched aralkyl, (un)substituted Ph; R2 = H, linear or branched lower alkyl; R3 = linear or branched alkyl, linear or branched alkenyl, linear or branched alkoxy, linear or branched alkenyloxy, linear or branched aralkyl, (un)substituted Ph] are useful as tumor promoter inhibitors. Stigmasteryl acetate was oxidized by m-chloroperbenzoic acid and hydrolyzed with HClO4 to give 3.beta.-acetoxystigmast-22-en-5.alpha.,6.beta.-diol (II). Oxidn. of II with pyridinium chlorochromate in the presence of Al2O3, followed by protection of the 6-position by ethylenedioxy group gave 3.beta.-acetoxy-6,6-ethylenedioxystigmast-22-en-5.alpha.-ol, which was subjected to ozonolysis in MeOH-CH2Cl2-pyridine to give bisnorcholan-22-al (III). Deprotection of III by hydrazine hydrate and KOH in ethylene glycol gave 3.beta.,5.alpha.-dihydroxy-23,24-bisnorcholan-6-one (YS-149) (IV). IV (at 1000 times excess) inhibited the binding of labeled 12-O-tetradecanoylphorbol 13-acetate (TPA) to cytosolic-nuclear tumor promoter-specific binding protein or protein kinase C by 48% or 0%, resp.

IT **156473-17-5P 161036-15-3P 161036-18-6P**
161036-19-7P 161106-46-3P 161106-47-4P
161106-48-5P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(steroids as tumor promoter inhibitors, and their prepn.)
RN 156473-17-5 CAPLUS
CN Pregn-5-en-20-ol, 3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

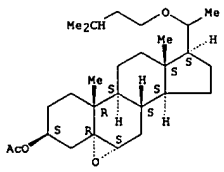
Absolute stereochemistry.



RN 161036-15-3 CAPLUS

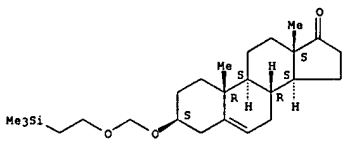
L28 ANSWER 28 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
CN Pregnan-3-ol, 5,6-epoxy-20-(3-methylbutoxy)-, acetate, (3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



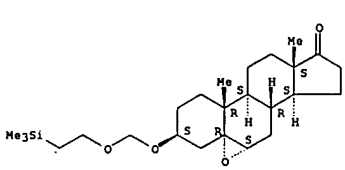
RN 161036-18-6 CAPLUS
CN Androst-5-en-17-one, 3-[[2-(trimethylsilyl)ethoxy]methoxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



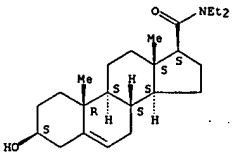
RN 161036-19-7 CAPLUS
CN Androstan-17-one, 5,6-epoxy-3-[[2-(trimethylsilyl)ethoxy]methoxy]-, (3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 161106-46-3 CAPLUS
CN Silane, (1,1-dimethylethyl)dimethyl[[(3.beta.)-20-(3-methylbutoxy)pregn-5-en-3-yl]oxy]- (9CI) (CA INDEX NAME)

L28 ANSWER 31 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



L28 ANSWER 32 OF 38 CAPLUS COPYRIGHT 2003 ACS

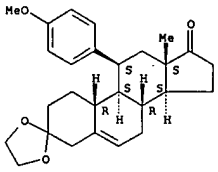
ACCESSION NUMBER: 1994:509371 CAPLUS
DOCUMENT NUMBER: 121:109371
TITLE: Synthesis and biological activity of 17-chloro-16(17)-unsaturated D-homo antiprogestins
AUTHOR(S): Schwede, Wolfgang; Cleve, Arwed; Neef, Guenter; Ottow, Eckhard; Stoeckemann, Klaus; Wiechert, Rudolf
CORPORATE SOURCE: Res. Lab., Schering AG, Berlin, Germany
SOURCE: Steroids (1994), 59(3), 176-80
CODEN: STEDAM; ISSN: 0039-128X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 121:109371

AB An efficient approach to 17-chloro-16(17)-unsatd. D-homo antiprogestins I (Y = Ac, 3-pyridyl) is described. The key steps of the synthesis are a ring-expansion via dichlorocarbene addn. to 17-silyl enol ether II (TBDMS = tert-butyldimethylsilyl) to give D-homosteroid III and a palladium-catalyzed coupling of 11.beta.-(4-aryltriflate) IV with tributyl(1-ethoxyethenyl)stannane or diethyl(3-pyridinyl)borane to give, after deketalization, I (Y = Ac and 3-pyridyl, resp.). The new progesterone antagonists were tested for their biol. activities and compared to those of know antiprogestins.

IT **139297-98-6**
RL: **RCT (Reactant)**; RACT (Reactant or reagent)
(demethylation of)

RN 139297-98-6 CAPLUS
CN Estr-5-ene-3,17-dione, 11-(4-methoxyphenyl)-, cyclic 3-(1,2-ethanediyl acetal), (11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

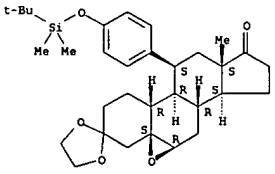


IT **156352-59-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and hydride redn. of)

RN 156352-59-9 CAPLUS
CN Estrane-3,17-dione, 11-[4-[[(1,1-dimethylethyl)dimethylsilyl]oxy]phenyl]-5,6-epoxy-, cyclic 3-(1,2-ethanediyl acetal), (5.beta.,6.beta.,11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

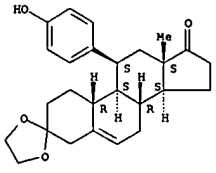
L28 ANSWER 32 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT **139298-03-6P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and silylation of, with tert-butyldimethylsilyl chloride)

RN 139298-03-6 CAPLUS
CN Estr-5-ene-3,17-dione, 11-(4-hydroxyphenyl)-, cyclic 3-(1,2-ethanediyl acetal), (11.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 33 OF 38 CAPLUS COPYRIGHT 2003 ACS

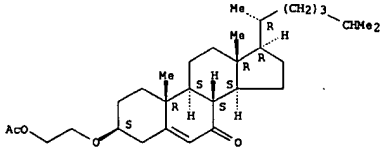
ACCESSION NUMBER: 1994:400454 CAPLUS
DOCUMENT NUMBER: 121:454
TITLE: Sterylcellosolves - new inhibitors of cholesterol biosynthesis in rabbit hepatocytes
AUTHOR(S): Misharin, Alexander Yu.; Malugin, Alexander V.; Steinschneider, Alexander Ya.; Kosykh, Vladimir A.; Novikov, Dmitry K.
CORPORATE SOURCE: Inst. Exp. Cardiol., Cardiol. Res. Cent., Moscow, Russia
SOURCE: Medicinal Chemistry Research (1993), (7), 451-8
CODEN: MCREEB; ISSN: 1054-2523
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Sterylcellosolves such as I-III were prepd. and inhibit cholesterol synthesis in isolated rabbit hepatocytes with I50 = 3.4 x 10-5 - 5.5 x 10-8 M.

IT **155252-29-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and alk. hydrolysis or redn. of)

RN 155252-29-2 CAPLUS
CN Cholest-5-en-7-one, 3-[2-(acetyloxy)ethoxy]-, (3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

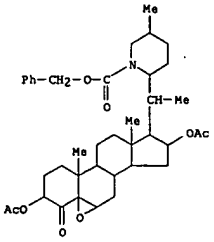


IT **155252-27-0P 155252-33-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and cholesterol biosynthesis in hepatocytes inhibition by)

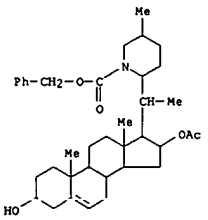
RN 155252-27-0 CAPLUS
CN Ethanol, 2-[[(3.beta.,5.alpha.,6.alpha.)-5,6-epoxycholestan-3-yl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L28 ANSWER 34 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

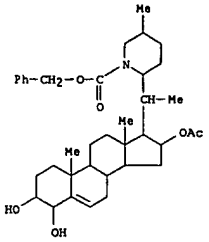


IT **144653-17-8P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and oxidn. of)
RN 144653-17-8 CAPLUS
CN 16,28-Secosolanid-5-ene-28-carboxylic acid, 16-(acetyloxy)-3-hydroxy-, phenylmethyl ester, (3.beta.,16.beta.,22.alpha.,25.beta.)- (9CI) (CA INDEX NAME)

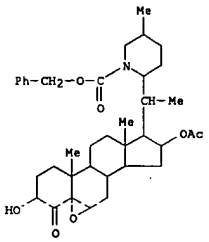


IT **144653-21-4P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and selective acetylation of)
RN 144653-21-4 CAPLUS
CN 16,28-Secosolanid-5-ene-28-carboxylic acid, 16-(acetyloxy)-3,4-dihydroxy-, phenylmethyl ester, (3.beta.,4.alpha.,16.beta.,22.alpha.,25.beta.)- (9CI) (CA INDEX NAME)

L28 ANSWER 34 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

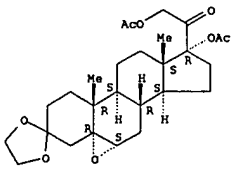


IT **144653-23-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 144653-23-6 CAPLUS
CN 16,28-Secosolanidane-28-carboxylic acid, 16-(acetyloxy)-5,6-epoxy-3-hydroxy-4-oxo-, phenylmethyl ester, (3.beta.,16.beta.,22.alpha.,25.beta.)- (9CI) (CA INDEX NAME)



L28 ANSWER 35 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1993:39247 CAPLUS
DOCUMENT NUMBER: 118:39247
TITLE: Incorporation of fluorine at position 6 of 17.alpha.-hydroxy-20-ketopregnanes. Synthesis of 6.alpha.-fluorocortexolone
AUTHOR(S): Ryakhovskaya, M. I.; Popova, E. V.; Alekseeva, L. M.; Grinenko, G. S.
CORPORATE SOURCE: TSNLS, VNIKhFI, Moscow, Russia
SOURCE: Khimiko-Farmatsevticheskii Zhurnal (1992), 26(6), 65-8
CODEN: KHFZAN; ISSN: 0023-1134
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 118:39247
AB Epoxidn. of 17.alpha.-hydroxyprogesterone I with monoperoxyphthalic acid gave 78% epoxide II which was fluorinated by HF to give 6-fluoro deriv. III. The latter was dehydrated in CF3CO2H-AcOH to give 94% enone IV which was epimerized in HCl. Subsequent sequential treatment with iodide and KOAc gave 64% hydroxyacetate (cortexolone deriv.) V. An alternative method for prepn. of the iodoacetate is also described.
IT **106545-20-4P 124113-12-8P 145013-91-8P**
145013-93-0P
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and deketalization of)
RN 106545-20-4 CAPLUS
CN Pregnane-3,20-dione, 17,21-bis(acetyloxy)-5,6-epoxy-, cyclic 3-(1,2-ethanediyl acetal), (5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

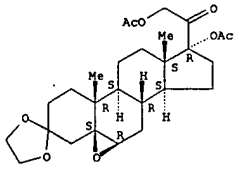
Absolute stereochemistry.



RN 124113-12-8 CAPLUS
CN Pregnane-3,20-dione, 17,21-bis(acetyloxy)-5,6-epoxy-, cyclic 3-(1,2-ethanediyl acetal), (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

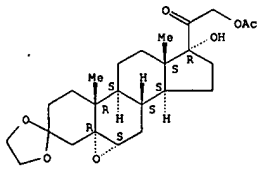
Absolute stereochemistry.

L28 ANSWER 35 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



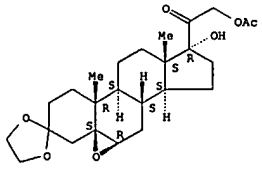
RN 145013-91-8 CAPLUS
CN Pregnane-3,20-dione, 21-(acetyloxy)-5,6-epoxy-17-hydroxy-, cyclic 3-(1,2-ethanediyl acetal), (5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 145013-93-0 CAPLUS
CN Pregnane-3,20-dione, 21-(acetyloxy)-5,6-epoxy-17-hydroxy-, cyclic 3-(1,2-ethanediyl acetal), (5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

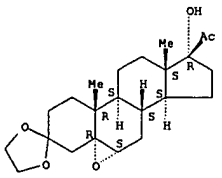
Absolute stereochemistry.



IT **145013-86-1P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. and fluorination by hydrofluoric acid)
RN 145013-86-1 CAPLUS
CN Pregnane-3,20-dione, 5,6-epoxy-17-hydroxy-, cyclic 3-(1,2-ethanediyl

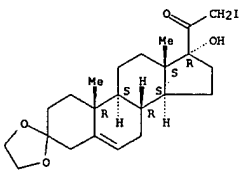
L28 ANSWER 35 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
acetal), (5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



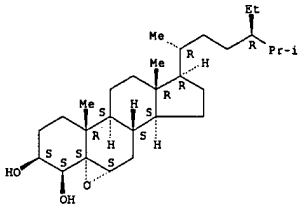
IT **145013-88-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and reaction with potassium acetate)
RN 145013-88-3 CAPLUS
CN Pregn-5-ene-3,20-dione, 17-hydroxy-21-iodo-, cyclic 3-(1,2-ethanediyl acetal), (5.alpha.,6.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



L28 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1992:255868 CAPLUS
DOCUMENT NUMBER: 116:255868
TITLE: Synthesis of 3.beta.,4.beta.-dihydroxy-6-oxo steroids from .beta.-sitosterol
AUTHOR(S): Kovganko, N. V.; Kashkan, Zh. N.
CORPORATE SOURCE: Inst. Bioorg. Khim., Ufa, USSR
SOURCE: Zhurnal Organicheskoi Khimii (1991), 27(9), 1896-900
CODEN: ZORKAE; ISSN: 0514-7492
DOCUMENT TYPE: Journal
LANGUAGE: Russian
OTHER SOURCE(S): CASREACT 116:255868
AB Allylic oxidn. of .beta.-sitosterol by SeO2 gave dihydroxy steroid I which was epoxidized by m-ClC6H4C(O)OOH to give 44% epoxide II and 28% epoxide III. Rearrangement of II with CF3CO2H gave 74% dihydroxy deriv. IV; acetylation of III by Ac2O gave 63% 3-acetate.
IT **141602-55-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and acetylation of)
RN 141602-55-3 CAPLUS
CN Stigmastane-3,4-diol, 5,6-epoxy-, (3.beta.,4.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

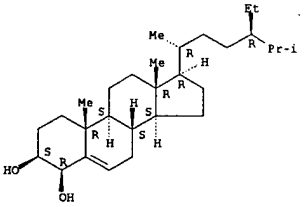
Absolute stereochemistry.



IT **141602-53-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and epoxidn. of)
RN 141602-53-1 CAPLUS
CN Stigmast-5-ene-3,4-diol, (3.beta.,4.beta.)- (9CI) (CA INDEX NAME)

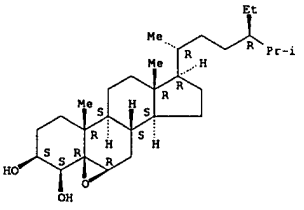
Absolute stereochemistry.

L28 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT **141602-54-2P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and rearrangement of)
RN 141602-54-2 CAPLUS
CN Stigmastane-3,4-diol, 5,6-epoxy-, (3.beta.,4.beta.,5.beta.,6.beta.)- (9CI) (CA INDEX NAME)

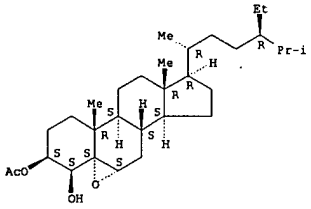
Absolute stereochemistry.



IT **141602-56-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(prepn. of)
RN 141602-56-4 CAPLUS
CN Stigmastane-3,4-diol, 5,6-epoxy-, 3-acetate, (3.beta.,4.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

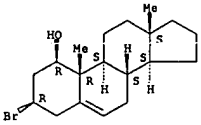
Absolute stereochemistry.

L28 ANSWER 36 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



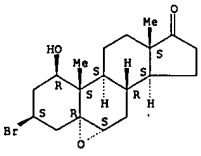
L28 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:536481 CAPLUS
DOCUMENT NUMBER: 115:136481
TITLE: Steroids. CCCLVIII. Revision of the structure of 3-methoxy-14.alpha.-hydroxy-D-homo-1,3,5(10)-estratrien-17a-one. A simple proton NMR method for the determination of configuration of the hydroxy group in position 5 and/or 14 of the D-homo-steroid skeleton
AUTHOR(S): Budesinsky, Milos; Kasal, Alexander; Prochazka, Zelimir; Huynh Kim Thoa; Vasickova, Sona; Kocovsky, Pavel
CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague, 166 10, Czech.
SOURCE: Collection of Czechoslovak Chemical Communications (1991), 56(7), 1512-24
CODEN: CCCCAK; ISSN: 0010-0765
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Eignerova and Prochazka found in 1974 the cotton effect value for 3-methoxy-14.alpha.-hydroxy-D-homo-1,3,5(10)-estratrien-17a-one I to be .DELTA..epsilon. - 2.76. Calcn. of the .DELTA..epsilon. value for this compd. led, however, to a substantially lower value, which suggested the hypothesis that the compd. was in fact rather an epimer with the hydroxy group in 14.beta.-position. This hypothesis was studied by means of 1H NMR spectra of synthetic models, using the changes of the chem. shifts of angular methyls, induced by in situ acylation of the angular hydroxyl with an .alpha.- or .beta.-configuration with trichloroacetyl isocyanate (TAI). The obsd. TAI-acylation shifts on model compds. indicated the structure I with a 14.beta.-configuration of the hydroxyl group. Independent proof has been given by the synthesis of both 14-hydroxy epimers of I. A simple 1H NMR method is proposed for the detn. of configuration of the hydroxyl in position 5 of 14 of D-homosteroid skeleton.
IT **136035-71-7P**
RL: PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and epoxidn. and NMR and configuration of)
RN 136035-71-7 CAPLUS
CN Androst-5-en-1-ol, 3-bromo-, (1.beta.,3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



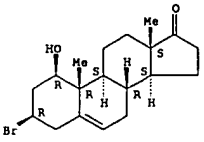
IT **136035-70-6P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and epoxidn. of)
RN 136035-70-6 CAPLUS

L28 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



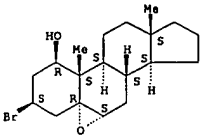
L28 ANSWER 37 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)
CN Androst-5-en-17-one, 3-bromo-1-hydroxy-, (1.beta.,3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **136035-73-9P**
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and redn. and configuration of)
RN 136035-73-9 CAPLUS
CN Androstan-1-ol, 3-bromo-5,6-epoxy-, (1.beta.,3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

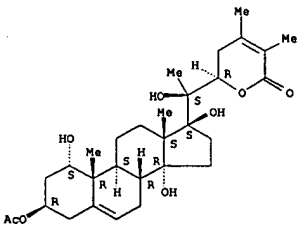


IT **136035-72-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(prepn. and redn. of, with lithium aluminum hydride)
RN 136035-72-8 CAPLUS
CN Androstan-17-one, 3-bromo-5,6-epoxy-1-hydroxy-, (1.beta.,3.beta.,5.alpha.,6.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L28 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 1991:102553 CAPLUS
DOCUMENT NUMBER: 114:102553
TITLE: Synthesis of the highly oxygenated ergostane type steroid (+)-withanolide E
AUTHOR(S): Perez-Medrano, Arturo; Grieco, Paul A.
CORPORATE SOURCE: Dep. Chem., Indiana Univ., Bloomington, IN, 47405, USA
SOURCE: Journal of the American Chemical Society (1991), 113(3), 1057-9
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 114:102553
AB The first synthesis of the highly oxygenated ergostane type steroid (+)-withanolide E (I) is reported. The synthesis commences with the known steroidal diacetate II which has been transformed into I via a sequence of reactions involving (a) a hetero Diels-Alder reaction for the incorporation of the C(14) .alpha.-hydroxyl group, (b) introduction of the C(17) .beta.-oriented hydroxy (c) stereospecific construction of the hydroxyl bearing carbons at C(10) and C(22), and (d) elaboration of the AB ring system possessing a .beta.-oriented epoxide at C(5), C(6).
IT **131759-48-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and Swern oxidn. of)
RN 131759-48-3 CAPLUS
CN Ergosta-5,24-dien-26-oic acid, 3-(acetyloxy)-1,14,17,20,22-pentahydroxy-, .delta.-lactone, (1.alpha.,3.beta.,17.alpha.,22R)- (9CI) (CA INDEX NAME)

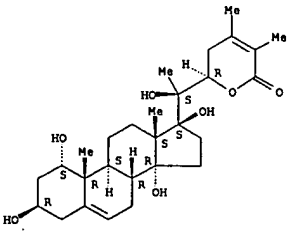
Absolute stereochemistry.



IT **131759-47-2P**
RL: PRP (Properties); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and acetylation and crystal structure of)
RN 131759-47-2 CAPLUS
CN Ergosta-5,24-dien-26-oic acid, 1,3,14,17,20,22-hexahydroxy-, .delta.-lactone, (1.alpha.,3.beta.,17.alpha.,22R)- (9CI) (CA INDEX NAME)

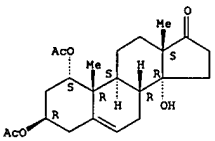
Absolute stereochemistry.

L28 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT 131759-41-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and deacetylation of)
RN 131759-41-6 CAPLUS
CN Androst-5-en-17-one, 1,3-bis(acetyloxy)-14-hydroxy-, (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

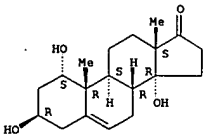
Absolute stereochemistry.



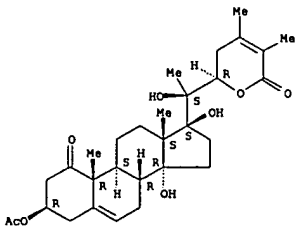
IT 131759-49-4P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. and sequential elimination reaction and epoxidn. of)
RN 131759-49-4 CAPLUS
CN Ergosta-5,24-dien-26-oic acid, 3-(acetyloxy)-14,17,20,22-tetrahydroxy-1-oxo-, .delta.-lactone, (3.beta.,17.alpha.,22R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L28 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)

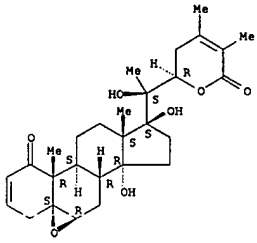


L28 ANSWER 38 OF 38 CAPLUS COPYRIGHT 2003 ACS (Continued)



IT 38254-15-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 38254-15-8 CAPLUS
CN Ergosta-2,24-dien-26-oic acid, 5,6-epoxy-14,17,20,22-tetrahydroxy-1-oxo-, .delta.-lactone, (5.beta.,6.beta.,17.alpha.,22R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 131759-42-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(prepn. of, as intermediate for withanolide)
RN 131759-42-7 CAPLUS
CN Androst-5-en-17-one, 1,3,14-trihydroxy-, (1.alpha.,3.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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=> d his

     (FILE 'HOME' ENTERED AT 09:00:53 ON 07 MAR 2003)

     FILE 'CASREACT' ENTERED AT 09:01:03 ON 07 MAR 2003
L1              STRUCTURE UPLOADED
L2            7 S L1
L3          154 S L1 FULL
L4          134 S L3 NOT PY>=2000

     FILE 'REGISTRY' ENTERED AT 09:03:39 ON 07 MAR 2003
L5          106 S DIOXIRANE

     FILE 'CASREACT' ENTERED AT 09:04:10 ON 07 MAR 2003
L6            3 S L3 AND L5
L7              STRUCTURE UPLOADED
L8          154 S L7 FULL
L9            3 S L8 AND L5
L10             STRUCTURE UPLOADED
L11          14 S L10 FULL

     FILE 'REGISTRY' ENTERED AT 09:11:50 ON 07 MAR 2003
L12             STRUCTURE UPLOADED
L13             STRUCTURE UPLOADED
L14             STRUCTURE UPLOADED
L15        1995 S L12 FULL
L16          50 S L13

     FILE 'CAPLUS' ENTERED AT 09:13:32 ON 07 MAR 2003
L17         858 S L15/PREP
L18         846 S L5/RCT
L19           8 S L17 AND L18
L20           0 S KETONE/FG.RCT

     FILE 'REGISTRY' ENTERED AT 09:23:18 ON 07 MAR 2003
L21             STRUCTURE UPLOADED
L22             STRUCTURE UPLOADED
L23             STRUCTURE UPLOADED
L24          50 S L22
L25       21091 S L22 FULL

     FILE 'CAPLUS' ENTERED AT 09:28:20 ON 07 MAR 2003
L26        1836 S L25/RCT
L27          55 S L17 AND L26
L28          38 S L27 NOT PY>=2000

=> file reg
COST IN U.S. DOLLARS                                SINCE FILE      TOTAL
                                                       ENTRY    SESSION
FULL ESTIMATED COST                                   179.98     953.82

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)          SINCE FILE      TOTAL
                                                       ENTRY    SESSION
CA SUBSCRIBER PRICE                                   -24.74     -40.49

FILE 'REGISTRY' ENTERED AT 09:34:03 ON 07 MAR 2003
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
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STRUCTURE FILE UPDATES: 5 MAR 2003 HIGHEST RN 497055-63-7
DICTIONARY FILE UPDATES: 5 MAR 2003 HIGHEST RN 497055-63-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> s l23
SAMPLE SEARCH INITIATED 09:34:11 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 171854 TO ITERATE

0.6% PROCESSED 1000 ITERATIONS 50 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 1000000

L29 50 SEA SSS SAM L23

=> s l23 full
FULL SEARCH INITIATED 09:34:17 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - >1,000,000 TO ITERATE

< 11.7% PROCESSED 400000 ITERATIONS 133593 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.10

FULL FILE PROJECTIONS: ONLINE **INCOMPLETE**
BATCH **INCOMPLETE**
PROJECTED ITERATIONS: EXCEEDS 1000000
PROJECTED ANSWERS: EXCEEDS 1000000

L30 133593 SEA SSS FUL L23

=> file caplus
COST IN U.S. DOLLARS SINCE FILE ENTRY TOTAL SESSION
FULL ESTIMATED COST 148.15 1101.97

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

	ENTRY	SESSION
CA SUBSCRIBER PRICE	0.00	-40.49

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FILE COVERS 1907 - 7 Mar 2003 VOL 138 ISS 11
FILE LAST UPDATED: 6 Mar 2003 (20030306/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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       2498896 RCT/RL
L31       5819 L30/RCT
                (L30 (L) RCT/RL)

=> d his

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     FILE 'CASREACT' ENTERED AT 09:01:03 ON 07 MAR 2003
L1              STRUCTURE UPLOADED
L2            7 S L1
L3          154 S L1 FULL
L4          134 S L3 NOT PY>=2000

     FILE 'REGISTRY' ENTERED AT 09:03:39 ON 07 MAR 2003
L5          106 S DIOXIRANE

     FILE 'CASREACT' ENTERED AT 09:04:10 ON 07 MAR 2003
L6            3 S L3 AND L5
L7              STRUCTURE UPLOADED
L8          154 S L7 FULL
L9            3 S L8 AND L5
L10             STRUCTURE UPLOADED
L11          14 S L10 FULL

     FILE 'REGISTRY' ENTERED AT 09:11:50 ON 07 MAR 2003
L12             STRUCTURE UPLOADED
L13             STRUCTURE UPLOADED
L14             STRUCTURE UPLOADED
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L15        1995 S L12 FULL
L16          50 S L13

     FILE 'CAPLUS' ENTERED AT 09:13:32 ON 07 MAR 2003
L17         858 S L15/PREP
L18         846 S L5/RCT
L19           8 S L17 AND L18
L20           0 S KETONE/FG.RCT

     FILE 'REGISTRY' ENTERED AT 09:23:18 ON 07 MAR 2003
L21             STRUCTURE UPLOADED
L22             STRUCTURE UPLOADED
L23             STRUCTURE UPLOADED
L24          50 S L22
L25       21091 S L22 FULL

     FILE 'CAPLUS' ENTERED AT 09:28:20 ON 07 MAR 2003
L26        1836 S L25/RCT
L27          55 S L17 AND L26
L28          38 S L27 NOT PY>=2000

     FILE 'REGISTRY' ENTERED AT 09:34:03 ON 07 MAR 2003
L29          50 S L23
L30      133593 S L23  FULL

     FILE 'CAPLUS' ENTERED AT 09:34:39 ON 07 MAR 2003
L31        5819 S L30/RCT

=> s l27 and l31
L32           0 L27 AND L31

=> d his

     (FILE 'HOME' ENTERED AT 09:00:53 ON 07 MAR 2003)

     FILE 'CASREACT' ENTERED AT 09:01:03 ON 07 MAR 2003
L1              STRUCTURE UPLOADED
L2            7 S L1
L3          154 S L1 FULL
L4          134 S L3 NOT PY>=2000

     FILE 'REGISTRY' ENTERED AT 09:03:39 ON 07 MAR 2003
L5          106 S DIOXIRANE

     FILE 'CASREACT' ENTERED AT 09:04:10 ON 07 MAR 2003
L6            3 S L3 AND L5
L7              STRUCTURE UPLOADED
L8          154 S L7 FULL
L9            3 S L8 AND L5
L10             STRUCTURE UPLOADED
L11          14 S L10 FULL

     FILE 'REGISTRY' ENTERED AT 09:11:50 ON 07 MAR 2003
L12             STRUCTURE UPLOADED
L13             STRUCTURE UPLOADED
L14             STRUCTURE UPLOADED
L15        1995 S L12 FULL
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L16          50 S L13

     FILE 'CAPLUS' ENTERED AT 09:13:32 ON 07 MAR 2003
L17         858 S L15/PREP
L18         846 S L5/RCT
L19           8 S L17 AND L18
L20           0 S KETONE/FG.RCT

     FILE 'REGISTRY' ENTERED AT 09:23:18 ON 07 MAR 2003
L21             STRUCTURE UPLOADED
L22             STRUCTURE UPLOADED
L23             STRUCTURE UPLOADED
L24          50 S L22
L25       21091 S L22 FULL

     FILE 'CAPLUS' ENTERED AT 09:28:20 ON 07 MAR 2003
L26        1836 S L25/RCT
L27          55 S L17 AND L26
L28          38 S L27 NOT PY>=2000

     FILE 'REGISTRY' ENTERED AT 09:34:03 ON 07 MAR 2003
L29          50 S L23
L30      133593 S L23  FULL

     FILE 'CAPLUS' ENTERED AT 09:34:39 ON 07 MAR 2003
L31        5819 S L30/RCT
L32           0 S L27 AND L31
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